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by JD Clayton

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Defects in nonlinear elastic crystals: differential geometry, finite kinematics, and second-order analytical solutions

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A differential geometric description of crystals with continuous distributions of lattice defects and undergoing potentially large deformations is presented. This description is specialized to describe discrete defects, i.e., singular defect distributions. Three isolated defects are considered in detail: the screw dislocation, the wedge disclination, and the point defect. New analytical solutions are obtained for elastic fields of these defects in isotropic solids of finite extent, whereby terms up to second order in strain, involving elastic constants up to third order, are retained in the stress components. The strain measure used in the nonlinear elastic potential – a symmetric function, expressed in material coordinates, of the inverse deformation gradient – differs from that used in previous solutions for crystal defects, and is thought to provide a more realistic depiction of mechanics of large deformation than previous theory involving third-order Lagrangian elastic constants and the Green strain tensor. For the screw dislocation and wedge disclination, effects of core pressure and/or possible contraction along the defect line are considered, and radial displacement contributions arise that are absent in the linear elastic solution, affecting dilatation. Stress components are shown to differ from those of linear elastic solutions near defect cores. Volume change from point defects is strongly affected by elastic nonlinearity.

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1 Introduction

Analysis of defects in deformable crystals has been a principal application of differential geometric methods to continuum mechanics of solids since the mid twentieth century. The earliest works linking continuous distributions of dislocations to geometric concepts are often attributed to Kondo, Bilby, Kröner, and co-workers [8,49,51]. Accompanying such works were development of a multiplicative decomposition of the deformation gradient [10,51] into lattice deformation, perhaps more often termed “elastic” deformation, and that due to dislocation glide, perhaps more often termed “plastic” deformation, and a linear connection with vanishing curvature whose torsion can be related to the dislocation density tensor [8,49,51]. These theories established a mathematical foundation for kinematics of finite deformation plasticity theory developed in subsequent decades [6,37,55,75,80].

Early geometric continuum theories admitting distributions of more general kinds of defects, including disclinations and point defects such as vacancies, substitutional atoms, or interstitial atoms [4,5,9,51,60] were introduced soon after dislocation theories. In some such descriptions [9,50,51] additional terms are incorporated multiplicatively into the deformation gradient to represent contributions of particular mechanisms distinct from dislocation slip (e.g., dilatation from point defects). The linear connection describing geometry of the defective crystal lattice may have curvature that can be related to disclination density and non-metricity that can be related to inhomogeneous distributions of point defects. General and rigorous geometric analyses of heterogeneous bodies undergoing finite incompatible deformation appeared around the same time [12,64,88].

More recent works have sought to extend or even reformulate continuum field theories of defective crystals applicable to the finite strain regime. Several works particularly relevant to developments in this paper are mentioned in what follows; a review of historic and more recent literature is beyond the present scope but can be found in [77]. In [1], an elastic-plastic dislocation field theory was developed that reduces to nonlinear elastic theory of distributed dislocations [91] in the time-independent limit. Gauge field theory has been applied to describe lattice defects [34,53,58], including single dislocations and dislocation distributions. Dislocations, disclinations, and point defects have recently been analyzed in theoretical frameworks incorporating Cartan’s moving frames [92–94]. Continuum dislocation theory has also been applied to shells undergoing finite deformation [3,96].

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In [19], a kinematic description was developed that accounts for simultaneous existence of dislocations, disclinations, and point defects. This treatment extended previous theory [5, 51, 60] by including statistically stored defects [i.e., dislocations (disclinations) with no net Burgers (Frank) vector] and incorporating a third term in the multiplicative decomposition associated with residual lattice deformation remaining in an element of material upon stress release, induced by microscopic elastic fields of defects within. Further developments on the origin of this third term in dislocated or twinned single crystals and polycrystals are reported in [13, 17, 22–24]. Thermodynamics and balance laws for a micropolar medium with dislocations and disclinations were developed in [25], and the geometric treatment was extended to dielectric solids with mobile vacancies and disclinations associated with domain walls [21]. Further derivations of fundamental geometric relations and potential applications in modern crystal plasticity theory are reported in the monograph [14].

In this paper a general theory for continuous defect distributions is presented first and then specialized to isolated defects in the Eulerian setting, differing from works by Kröner and Seeger [52] and Willis [91] that dealt only with dislocations in the Lagrangian setting. For elastic bodies containing dislocations, disclinations, and point defects, some parallels between continuous and discrete defect theories were noted by De Wit [31, 32], albeit restricted to linear theory, i.e., small deformation. Nonlinear theory developed in the present work extends [31, 32] by associating certain singular part(s) of total finite distortion with inelastic deformation due to isolated defects, making use of generalized functions [39] to address singular quantities.

Linear elasticity is typically deemed sufficient for representing elastic fields beyond some distance from the core of the defect. For defect densities that are not too large, the mean spacing between defects is great enough that stress fields can be addressed using linear elastic solutions. However, close to the core, strain component(s) from linear elastic solutions are quite large, rendering the linear analysis inaccurate [38, 81]. Furthermore, some physical features apparent in experiments and atomic simulation such as residual lattice dilatation [44, 76, 95] and phonon scattering [71] cannot be predicted by linear theory, but can be predicted using nonlinear elasticity.

Analytical solutions to nonlinear boundary value problems for crystals with individual defects can be considered relatively scarce relative to abundant linear elastic solutions. Exact analytical solutions appear to exist only for solids described by strain energy potentials that may be physically unrealistic for real crystals. Exact closed-form solutions can be obtained for incompressible elasticity, as has been demonstrated for the screw dislocation [1, 69, 92, 96]. It has been noted [38] that displacement fields of a screw dislocation and a wedge disclination are a subset of a larger family of controllable deformations for which universal solutions exist in incompressible isotropic elastostatics [89]. Incompressible constitutive models, by definition, cannot address residual elastic dilatation and hence are not physically realistic in this regard. Analytical solutions for wedge disclinations and point defects have been reported for materials obeying incompressible neo-Hookean elasticity [93, 94]. For compressible solids, several exact analytical solutions for dislocation and disclination configurations have been derived using finite strain measures [33, 96, 97], but the semi-linear energy potential used in these analyses may not address fully nonlinear behavior in typical crystalline metals and minerals. In particular, this semi-linear potential depends on only two elastic constants rather than the usual five for a second-order nonlinear hyperelastic and isotropic solid. An exact solution has also been derived for the screw dislocation in an isotropic solid with a nonlinear elastic potential depending on the small strain tensor [46].

Approximate analytical solutions have been found for solids obeying more physically realistic strain energy potentials. In such approaches, a nonlinear elastic potential is invoked, but higher-order products of displacement gradients entering the stress field are truncated above a certain order. The qualifier “second-order” is used here to denote an elasticity solution wherein stress depends quadratically on strain, with the elastic potential cubic in strain and including elastic constants of up to order three. A “first-order” solution denotes a linear stress-strain response and a quadratic elastic potential, i.e., usual linear elasticity.

Kröner and colleagues [52, 67] instituted a geometric stress function method for obtaining second-order accurate solutions for isotropic dislocated bodies obeying Murnaghan’s Eulerian elastic potential [61]. Stress fields were reported for dislocations in infinite bodies and in finite bodies with stress-free cores, for singular densities of edge and screw dislocations; this solution technique explicitly yields stresses but not displacements. Seeger and Mann [72] derived a solution for the screw dislocation with a hollow (stress-free) core using an isotropic second-order Lagrangian analysis, i.e., strain energy potential in terms of Green strain with up to third-order elastic constants. Willis [91] formulated an iterative procedure involving Green’s functions for infinite anisotropic bodies with dislocations, but did not address core boundary conditions. An approximate solution for an edge dislocation in an infinite medium obeying isotropic Lagrangian elasticity was reported [48], following general techniques for analysis of planar second-order nonlinear elastic problems [2]. Teodosiu and Soós [81, 82] formalized a general iterative procedure¹ for analysis of dislocations in nonlinear elasticity, similar to those implemented in [38, 72, 73, 91], demonstrating certain uniqueness properties of first- and second-order solutions. A

¹ Such iterative methods for solution of nonlinear elastic problems were apparently first reported by Signorini [74] and were applied intuitively to a number of problems by Murnaghan [62].

second-order solution for the isolated screw dislocation in a finite cylinder with core pressure was derived in [81], incorporating Eulerian coordinates and the Lagrangian energy potential mentioned above. Advantages of Eulerian coordinates over Lagrangian coordinates have been discussed [83]. More recently, gauge theory was used to obtain a second-order solution for a screw dislocation in isotropic Eulerian elasticity [58].

For an isolated wedge disclination, a solution incorporating both Eulerian coordinates and Murnaghan's Eulerian potential was derived [68, 86], but core pressure was not addressed. For an isolated point defect, Seeger and Mann [72] extended the approximate second-order Lagrangian analysis of Murnaghan [62], who treated a thick spherical shell with pressurized interior and exterior boundaries. In this work [72], both the defect and medium were treated as elastic bodies with potentially different second- and third-order elastic constants; see also [57] that addresses related nonlinear elastic problems including interactions among spherical inclusions.

As inferred from above, second-order solutions involve elastic constants of orders two and three. These approximate solutions are usually justified by the limitation that complete elastic constants of order four have rarely been available for real materials, and solutions of higher order would require knowledge of fourth-order constants. Possible relationships between fourth-order constants and geometric features of the edge dislocation core have been noted [47]. Longitudinal fourth-order constants can be inferred from shock compression data [16], and Density Functional Theory (DFT) can be used to predict fourth-order constants [63], though accuracy of such predictions is uncertain. Regardless, when strains become large enough that third-order elastic constants are insufficient, it becomes prudent to study core fields using atomic simulation [20, 26, 27, 76] rather than traditional continuum elasticity. Nonlocal, strain gradient, and/or gauge theories [53, 58] of continua may also enable a physically realistic description (e.g., smoothed or non-singular) of defect cores. Second-order solutions derived later in this work are intended for regimes and materials where a third-order elastic potential is accurate and exclude the (singular) defect core. Higher-order gradients of deformation (e.g., as treated in a general constitutive formalism in [79]) are not incorporated in the elastic potential used here.

Previous second-order elastic analyses of lattice defects mentioned above have either used a Green Lagrangian elastic potential $\bar{W}(\mathbf{E})$ [14, 62, 87] or Murnaghan's Eulerian potential $\tilde{W}(e)$ [61], the latter restricted to isotropic solids. [Precisely, letting \mathbf{F} denote the two-point deformation gradient tensor, Green strain is $\mathbf{E} = \frac{1}{2}(\mathbf{F}^T \mathbf{F} - \mathbf{1})$ and Almansi strain is $\mathbf{e} = \frac{1}{2}(\mathbf{1} - \mathbf{F}^{-T} \mathbf{F}^{-1})$.] In contrast, new nonlinear elastic solutions derived in the present work incorporate the less often encountered Eulerian strain energy potential $\hat{W}(\mathbf{D})$, where $\mathbf{D} = \frac{1}{2}(\mathbf{1} - \mathbf{F}^{-1} \mathbf{F}^{-T})$. Symmetric tensor \mathbf{D} is termed an "Eulerian" strain in material coordinates [28], is invariant under rigid rotations of the spatial coordinate frame, and was introduced by Thomsen [85] and soon thereafter Davies [29] for describing the nonlinear thermoelastic response of pressurized cubic crystals. Unlike \tilde{W} , potential \hat{W} can be applied to anisotropic solids [66, 90]. This model has demonstrated greater intrinsic stability [43] at large shear and compression than usual Lagrangian elasticity incorporating \bar{W} that tends towards instability at large uniaxial compression [16]. It is also more accurate for addressing the response of most crystalline solids under hydrostatic compression, whereby at second order it degenerates to the Birch-Murnaghan equation-of-state [11, 84] for cubic crystals and isotropic media. In contrast, second-order Lagrangian theory tends to underestimate pressure at large compression [45]. Improved accuracy of \hat{W} over \bar{W} for describing hydrostatic compression of lower symmetry crystals has been reported [66, 90]. The nonlinear elastic response of diamond under finite strain predicted by DFT [63] is also better represented by Eulerian elasticity incorporating \hat{W} than Lagrangian elasticity incorporating \bar{W} , with elastic constants of up to order four considered in each representation. Recent analysis [16] has empirically demonstrated other advantages of Eulerian theory (based on \hat{W}) over Lagrangian theory for homogeneous static compression and homogeneous shear of representative cubic or isotropic solids with Cauchy symmetry of third-order elastic constants. For crystals of lower symmetry (e.g., quartz and sapphire) subjected to uniaxial shock compression, advantages of Eulerian over Lagrangian theory were less evident. Solutions derived later in the present paper are the first known for dislocations, disclinations, and point defects incorporating elastic potential $\hat{W}(\mathbf{D})$.

Eulerian potential $\hat{W}(\mathbf{D})$ is used to obtain new second-order analytical solutions to three discrete defect problems in the present paper, which is structured as follows. In Sect. 2, continuum defect theory is concisely reviewed, refining certain aspects of earlier work [14, 19]. In Sect. 3, the screw dislocation is analyzed. In Sect. 4, the wedge disclination is analyzed. In Sect. 5, the point defect is analyzed. For each kind of defect, it is shown how continuum field theory with a multiplicative decomposition of the deformation gradient and additive decomposition of a linear connection can be applied to the limiting case of a singular defect density. A second-order elastic analysis is used in each case, with solutions expressed in Eulerian coordinates. For the dislocation and disclination, core pressure is included. All three solutions are believed to be new. Representative calculations demonstrate differences between nonlinear and linear elastic solutions. Conclusions follow in Sect. 6. Appendices A and B provide supporting discussion on finite deformation in cylindrical and spherical coordinate systems used in the derivations, while Appendix C describes nonlinear elastic potentials and associated second- and third-order elastic constants and clarifies differences among several nonlinear elastic theories. Direct tensor notation [64, 78] and coordinate notation of tensor calculus [36, 70, 77] are used interchangeably as needed.

2 Continuous defect distributions

2.1 General continuum theory

Consider a solid body whose unstressed reference configuration \mathfrak{B}_0 is perfectly crystalline and simply connected. At some time t , this body in its current configuration representation \mathfrak{B} may contain defects and may support stresses, both residual and due to externally applied traction. Deformed body \mathfrak{B} is assumed to remain simply connected in the continuum theory, and defects are characterized by spatially continuous density functions. A local volume element is associated with a material particle at position \mathbf{X} in three-dimensional Euclidean space and is mapped to position \mathbf{x} at time t . This element may contain a number of defects such as dislocations, the product of whose number and Burgers vector remains finite [91].

Henceforth attention is restricted to a deformed configuration at a single time t , such that the description becomes time-independent. Let $\{X^A\}$ and $\{x^a\}$ denote coordinate charts covering \mathfrak{B}_0 and \mathfrak{B} , respectively. The following one-to-one and presumably three times differentiable functions exist:

$$\mathbf{x} = \mathbf{x}(\mathbf{X}), \quad \mathbf{X} = \mathbf{X}(\mathbf{x}). \quad (2.1)$$

Letting $\partial_A(\cdot) = \partial(\cdot)/\partial X_A$ and $\partial_a(\cdot) = \partial(\cdot)/\partial x_a$, natural basis vectors are

$$\mathbf{G}_A(\mathbf{X}) = \partial_A \mathbf{X}, \quad \mathbf{g}_a(\mathbf{x}) = \partial_a \mathbf{x}. \quad (2.2)$$

The deformation gradient and its inverse are

$$\mathbf{F} = \partial_A \mathbf{x} \otimes \mathbf{G}^A, \quad \mathbf{F}^{-1} = \partial_a \mathbf{X} \otimes \mathbf{g}^a, \quad (2.3)$$

where, with $G_{AB}(\mathbf{X})$ and $g_{ab}(\mathbf{x})$ referential and spatial metric tensor components,

$$\mathbf{G}_A = G_{AB} \mathbf{G}^B = (\mathbf{G}_A \cdot \mathbf{G}_B) \mathbf{G}^B, \quad \mathbf{g}_a = g_{ab} \mathbf{g}^b = (\mathbf{g}_a \cdot \mathbf{g}_b) \mathbf{g}^b. \quad (2.4)$$

In component form,

$$F^a_{\cdot A} = \partial_A x^a, \quad F^{-1A}_{\cdot a} = \partial_a X^A. \quad (2.5)$$

Conventional gradient operators on \mathfrak{B}_0 and \mathfrak{B} are denoted by ∇_0 and ∇ . For example, letting \mathbf{V} and \mathbf{v} denote material and spatial vector fields, covariant derivatives are

$$\nabla_0 \mathbf{V} = \partial_B \mathbf{V} \otimes \mathbf{G}^B = (\partial_B V^A + \Gamma_{BC}^A V^C) \mathbf{G}_A \otimes \mathbf{G}^B, \quad (2.6)$$

$$\nabla \mathbf{v} = \partial_b \mathbf{v} \otimes \mathbf{g}^b = (\partial_b v^a + \gamma_{bc}^{*a} v^c) \mathbf{g}_a \otimes \mathbf{g}^b, \quad (2.7)$$

where Levi-Civita connection coefficients

$$\Gamma_{BC}^{*A} = \frac{1}{2} G^{AD} (\partial_B G_{CD} + \partial_C G_{BD} - \partial_D G_{BC}), \quad \gamma_{bc}^{*a} = \frac{1}{2} g^{ad} (\partial_b g_{cd} + \partial_c g_{bd} - \partial_d g_{bc}). \quad (2.8)$$

From the properties of mappings in (2.1) and presumed positivity of local volume elements in \mathfrak{B}_0 and \mathfrak{B} in right-handed coordinate systems, restrictions $\det \mathbf{F} > 0$ and $\det \mathbf{F}^{-1} > 0$ emerge. Since $\{X^A\}$ and $\{x^a\}$ are holonomic, $\partial_A[\partial_B(\cdot)] = \partial_B[\partial_A(\cdot)]$ and $\partial_a[\partial_b(\cdot)] = \partial_b[\partial_a(\cdot)]$, and since the body is embedded in Euclidean space, Riemann-Christoffel curvature tensors constructed from (2.8) vanish identically. From (2.5) and symmetry of connection coefficients in (2.8), the following local compatibility (i.e., null curl) conditions apply:

$$\nabla_0 \times \mathbf{F} = \mathbf{0}, \quad \nabla \times (\mathbf{F}^{-1}) = \mathbf{0}. \quad (2.9)$$

For defective crystals a multiplicative decomposition of \mathbf{F} is invoked [10, 14, 51]:

$$\mathbf{F} = \mathbf{F}^L \mathbf{F}^P, \quad F^a_{\cdot A} = F^{L\ a}_{\cdot A} F^{P\ \alpha}_{\cdot A}. \quad (2.10)$$

Lattice deformation \mathbf{F}^L accounts for elastic stretch (recoverable and/or residual) and rotation; plastic deformation \mathbf{F}^P accounts for slip from dislocations that preserves the lattice structure [9, 10]. Both fields are assumed invertible, with positive determinants, and at least twice differentiable with respect to X^A and x^a . Neither, however, is necessarily integrable to a motion nor satisfies conditions analogous to (2.9); i.e., lattice and plastic deformation tensors are generally anholonomic. Thus, the intermediate configuration \mathfrak{B} of the body implied by (2.10) cannot be embedded in three-dimensional Euclidean space [15, 41]. Letting $\{\mathbf{g}_\alpha\}$ denote a generally non-coordinate basis, with reciprocal basis $\{\mathbf{g}^\alpha\}$,

$$\mathbf{F}^L = F^{L\ a}_{\cdot \alpha} \mathbf{g}_a \otimes \mathbf{g}^\alpha, \quad \mathbf{F}^P = F^{P\ \alpha}_{\cdot A} \mathbf{g}_\alpha \otimes \mathbf{G}^A. \quad (2.11)$$

Introduced at each point $\mathbf{X} \in \mathfrak{B}_0$ is a triad of undeformed lattice director vectors $\{\mathbf{d}_A\}$ and their reciprocals $\{\mathbf{d}^A\}$, such that $\langle \mathbf{d}^A, \mathbf{d}_B \rangle = \delta_B^A$ with $\langle \cdot, \cdot \rangle$ a scalar product. Referential director vectors are orthonormal: $\mathbf{d}_A \cdot \mathbf{d}_B = \delta_{AB}$ and $\mathbf{d}_A = \delta_{AB} \mathbf{d}^B$. In crystal structures with cubic, tetragonal, or orthorhombic symmetry, a referential lattice vector can be assigned parallel to each edge of the unit cell. Also introduced at each $\mathbf{x} \in \mathfrak{B}$ is a triad of deformed lattice directors $\{\mathbf{d}_a\}$ and their reciprocals $\{\mathbf{d}^a\}$, such that $\langle \mathbf{d}^a, \mathbf{d}_b \rangle = \delta_b^a$. Deformed director vectors are generally neither orthogonal nor of unit length:

$$\mathbf{d}^a = F^{\mathbf{L} \ a}_{\cdot \alpha} \delta_{\alpha}^A \mathbf{d}^A, \quad \mathbf{d}_a = F^{\mathbf{L}-1 \alpha}_{\cdot a} \delta_{\alpha}^A \mathbf{d}_A. \quad (2.12)$$

The metric tensor associated with the deformed lattice is

$$\mathbf{d} = (\mathbf{d}_a \cdot \mathbf{d}_b) \mathbf{g}^a \otimes \mathbf{g}^b = \mathbf{F}^{\mathbf{L}-\mathbf{T}} \mathbf{F}^{\mathbf{L}-1}. \quad (2.13)$$

In components, this metric and its inverse are

$$d_{ab} = F^{\mathbf{L}-1 \alpha}_{\cdot a} \delta_{\alpha \beta} F^{\mathbf{L}-1 \beta}_{\cdot b}, \quad d^{ab} = F^{\mathbf{L} \ a}_{\cdot \alpha} \delta^{\alpha \beta} F^{\mathbf{L} \ b}_{\cdot \beta}, \quad (2.14)$$

leading to

$$\mathbf{d}_a = d_{ab} \mathbf{d}^b, \quad \mathbf{d}^a = d^{ab} \mathbf{d}_b. \quad (2.15)$$

Components of lattice deformation can be inferred from scalar products of referential and deformed directors:

$$F^{\mathbf{L} \ a}_{\cdot \alpha} = \langle \mathbf{d}^a, \mathbf{d}_A \rangle \delta_{\alpha}^A, \quad F^{\mathbf{L}-1 \alpha}_{\cdot a} = \langle \mathbf{d}_a, \mathbf{d}^A \rangle \delta_{\alpha}^A, \quad (2.16)$$

and if a coordinate frame on \mathfrak{B} is chosen parallel to the reference lattice such that $\{\mathbf{g}_{\alpha}\} \rightarrow \{\mathbf{d}_A \delta_{\alpha}^A\}$,

$$\mathbf{F}^{\mathbf{L}} = \mathbf{g}_a \otimes \mathbf{d}^a, \quad \mathbf{F}^{\mathbf{L}-1} = \mathbf{d}_a \otimes \mathbf{g}^a. \quad (2.17)$$

In the continuum field theory of defects, the geometry of the (possibly defective) crystal lattice is characterized by covariant derivatives of the spatial lattice director fields, defined as [14, 19, 60]

$$\hat{\nabla}_b \mathbf{d}_a = \partial_b \mathbf{d}_a - \hat{\Gamma}_{ba}^{\cdot c} \mathbf{d}_c, \quad \hat{\nabla}_b \mathbf{d}^a = \partial_b \mathbf{d}^a + \hat{\Gamma}_{bc}^{\cdot a} \mathbf{d}^c. \quad (2.18)$$

A complete description of the deformed lattice is given by the fields $\{\mathbf{d}_a\}$ and $\{\hat{\nabla} \mathbf{d}_a\}$, where $a = 1, 2, 3$. From (2.16) and (2.18), this description is furnished by knowledge of the fields $\mathbf{F}^{\mathbf{L}}$ (up to 9 components) and $\hat{\Gamma}$ (up to 27 components) which are available at each point $\mathbf{x} \in \mathfrak{B}$, or equivalently at each point $\mathbf{X} \in \mathfrak{B}_0$ since \mathbf{x} and \mathbf{X} are one-to-one in (2.1). An additive decomposition of connection coefficients associated with $\hat{\nabla}$, assumed at least once differentiable over \mathfrak{B} , is invoked [14, 19, 60]:

$$\hat{\Gamma}_{bc}^{\cdot a} = \bar{\Gamma}_{bc}^{\cdot a} + Q_{bc}^{\cdot a}. \quad (2.19)$$

Coefficients $\bar{\Gamma}$ are spatial representations of those of the usual non-Riemannian connection of dislocation field theory, referred to as a “crystal connection” [54] in the context of nonlinear elastoplasticity or an example of a “Weitzenböck” connection in differential geometry [53, 92]:

$$\bar{\Gamma}_{bc}^{\cdot a} = F^{\mathbf{L} \ a}_{\cdot \alpha} \partial_b F^{\mathbf{L}-1 \alpha}_{\cdot c} = -F^{\mathbf{L}-1 \alpha}_{\cdot c} \partial_b F^{\mathbf{L} \ a}_{\cdot \alpha}. \quad (2.20)$$

The torsion tensor of (2.19) is

$$\hat{\mathbf{T}} = \hat{\Gamma}_{[bc]}^{\cdot a} \mathbf{g}^b \otimes \mathbf{g}^c \otimes \mathbf{g}_a, \quad \hat{T}_{bc}^{\cdot a} = \frac{1}{2} (\hat{\Gamma}_{bc}^{\cdot a} - \hat{\Gamma}_{cb}^{\cdot a}) = F^{\mathbf{L} \ a}_{\cdot \alpha} \partial_{[b} F^{\mathbf{L}-1 \alpha}_{\cdot c]} + Q_{[bc]}^{\cdot a}, \quad (2.21)$$

where indices in square brackets are skew. Verification is straightforward that the Riemann-Christoffel curvature tensor from (2.20) vanishes identically, meaning this connection is flat or integrable:

$$\begin{aligned} \bar{\mathbf{R}} &= 2(\partial_{[b} \bar{\Gamma}_{c]d}^{\cdot a} + \bar{\Gamma}_{[b|e|}^{\cdot a} \bar{\Gamma}_{c]d}^{\cdot e}) \mathbf{g}^b \otimes \mathbf{g}^c \otimes \mathbf{g}^d \otimes \mathbf{g}_a \\ &= 2F^{\mathbf{L} \ a}_{\cdot \alpha} \partial_{[b} \partial_{c]} F^{\mathbf{L}-1 \alpha}_{\cdot d} \mathbf{g}^b \otimes \mathbf{g}^c \otimes \mathbf{g}^d \otimes \mathbf{g}_a = \mathbf{0}. \end{aligned} \quad (2.22)$$

Indices in vertical bars are excluded from (anti)symmetry operations. The curvature tensor of (2.19) is [14, 70]

$$\begin{aligned}\hat{\mathbf{R}} &= 2(\partial_{[b}\hat{\Gamma}_{c]d}^{\bullet\bullet a} + \hat{\Gamma}_{[b|e|}^{\bullet\bullet a}\hat{\Gamma}_{c]d}^{\bullet\bullet e})\mathbf{g}^b \otimes \mathbf{g}^c \otimes \mathbf{g}^d \otimes \mathbf{g}_a \\ &= 2(\hat{\nabla}_{[b}Q_{c]d}^{\bullet\bullet a} + \hat{T}_{bc}^{\bullet\bullet e}Q_{ed}^{\bullet\bullet a} + Q_{[b|d|}^{\bullet\bullet e}Q_{c]e}^{\bullet\bullet a})\mathbf{g}^b \otimes \mathbf{g}^c \otimes \mathbf{g}^d \otimes \mathbf{g}_a,\end{aligned}\quad (2.23)$$

where

$$\hat{\nabla}_b Q_{cd}^{\bullet\bullet a} = \partial_b Q_{cd}^{\bullet\bullet a} + \hat{\Gamma}_{be}^{\bullet\bullet a} Q_{cd}^{\bullet\bullet e} - \hat{\Gamma}_{bc}^{\bullet\bullet e} Q_{ed}^{\bullet\bullet a} - \hat{\Gamma}_{bd}^{\bullet\bullet e} Q_{ce}^{\bullet\bullet a}.\quad (2.24)$$

Nonmetricity of connection (2.19) is

$$\hat{\nabla}_c d_{ab} = \partial_c d_{ab} - \hat{\Gamma}_{ca}^{\bullet\bullet e} d_{be} - \hat{\Gamma}_{cb}^{\bullet\bullet e} d_{ae} = -(Q_{ca}^{\bullet\bullet e} d_{eb} + Q_{cb}^{\bullet\bullet e} d_{ea}) = -2Q_{c(ab)},\quad (2.25)$$

where indices in parentheses are symmetric and d is used to lower indices of \mathbf{Q} . Covariant components of $\hat{\mathbf{R}}$ are

$$\hat{R}_{bcda} = \hat{R}_{bcd}^{\bullet\bullet e} d_{ea} = 2(\hat{\nabla}_{[b}Q_{c]da} + \hat{T}_{bc}^{\bullet\bullet e} Q_{eda} - Q_{[b|d|}^{\bullet\bullet e} Q_{c]ae}),\quad (2.26)$$

$$\hat{R}_{[bc](da)} = \hat{R}_{bc(a)d} = 2(\hat{\nabla}_{[b}Q_{c](da)} + \hat{T}_{bc}^{\bullet\bullet e} Q_{e(da)}),\quad (2.27)$$

$$\hat{R}_{[bc][da]} = -\hat{R}_{bc[ad]} = 2(\hat{\nabla}_{[b}Q_{c][da]} + \hat{T}_{bc}^{\bullet\bullet e} Q_{e[da]}) - Q_{b[d|}^{\bullet\bullet e} Q_{c|a]e} + Q_{c[d|}^{\bullet\bullet e} Q_{b|a]e}.\quad (2.28)$$

Curvature and non-metricity arise from \mathbf{Q} and vanish when $\hat{\Gamma} = \bar{\Gamma}$; nonmetricity further depends only on the symmetric part of \mathbf{Q} in (2.25).

Mathematical quantities associated with defect densities are now defined. The spatial dislocation density tensor is

$$\boldsymbol{\alpha} = -\hat{\mathbf{T}} : \boldsymbol{\epsilon} = \epsilon^{bcd} \hat{T}_{dc}^{\bullet\bullet a} \mathbf{g}_a \otimes \mathbf{g}_b,\quad (2.29)$$

where ϵ is the spatial permutation tensor. Usual dimensionless permutation symbols are $e_{abc} = e^{abc} = g^{-1/2} \epsilon_{abc} = g^{1/2} \epsilon^{abc}$ with $g = \det[\partial_a \mathbf{x} \cdot \partial_b \mathbf{x}]$. Let $(\cdot)^T$ denote the transpose of a second-order tensor. The spatial disclination density tensor is

$$\boldsymbol{\theta} = -\frac{1}{4}(\boldsymbol{\epsilon} : \hat{\mathbf{R}} : \boldsymbol{\epsilon})^T = \frac{1}{4} \epsilon^{acd} \epsilon^{bef} \hat{R}_{fed} \mathbf{g}_a \otimes \mathbf{g}_b.\quad (2.30)$$

Henceforth restricting nonmetricity as

$$Q_{a(bc)} = -\frac{1}{2} \hat{\nabla}_a d_{bc} = \Upsilon_a d_{bc}, \quad Q_{b(cd)} d^{da} = \frac{1}{2} d^{ad} (Q_{bcd} + Q_{bdc}) = \Upsilon_b \delta_c^a,\quad (2.31)$$

a vector quantity associated with point defects can be defined [14, 21]:

$$\boldsymbol{\vartheta} = -\nabla \times \boldsymbol{\Upsilon} = \boldsymbol{\epsilon} : \nabla \boldsymbol{\Upsilon} = \epsilon^{abc} \partial_c \Upsilon_b \mathbf{g}_a.\quad (2.32)$$

Inverting (2.29), (2.30), and (2.32) enables reconstruction of the torsion and curvature:

$$\hat{T}_{bc}^{\bullet\bullet a} = \frac{1}{2} \epsilon_{cbd} \alpha^{ad}, \quad \hat{R}_{ab[cd]} = \epsilon_{bae} \epsilon_{cdf} \theta^{fe}, \quad \hat{R}_{ab(cd)} = \epsilon_{bae} \vartheta^e d_{cd}.\quad (2.33)$$

Identify \mathfrak{B} as a manifold equipped with connection $\hat{\nabla}$. Let $\{\mathbf{u}, \mathbf{v}, \mathbf{w}\}$ be smooth vector fields on the tangent bundle of \mathfrak{B} . Then

$$(\hat{\nabla} \hat{\nabla} \mathbf{u}) : (\mathbf{v} \otimes \mathbf{w} - \mathbf{w} \otimes \mathbf{v}) = (\hat{\mathbf{R}} \mathbf{u} - 2\hat{\mathbf{T}} \hat{\nabla} \mathbf{u}) : (\mathbf{v} \otimes \mathbf{w}),\quad (2.34)$$

or in a coordinate chart $\{x^a\}$ [70],

$$\hat{\nabla}_{[b} \hat{\nabla}_{c]} u^a = \frac{1}{2} \hat{R}_{bcd}^{\bullet\bullet a} u^d - \hat{T}_{bc}^{\bullet\bullet d} \hat{\nabla}_d u^a.\quad (2.35)$$

This identity can be used to prove that under a “Cartan displacement”, a vector \mathbf{u} undergoes a first-order (with respect to transported distance $d\mathbf{x}$) change upon parallel transport about an infinitesimal circuit dc of the form $\mathbf{u} \rightarrow \mathbf{u} + \delta \mathbf{u}$, where [60, 70, 89]

$$\delta \mathbf{u} = -(\frac{1}{2} \hat{R}_{bcd}^{\bullet\bullet a} u^d + \hat{T}_{bc}^{\bullet\bullet a}) da^{bc} \mathbf{g}_a.\quad (2.36)$$

The oriented area element enclosed by dc has magnitude da , unit normal \mathbf{n} , and obeys

$$d\mathbf{a} = da^{bc} \mathbf{g}_b \otimes \mathbf{g}_c = \epsilon^{bca} n_a da \mathbf{g}_b \otimes \mathbf{g}_c, \quad n_a da = \frac{1}{2} \epsilon_{abc} da^{bc}. \quad (2.37)$$

From (2.36), $\delta \mathbf{u}$ consists of two parts: one proportional to \mathbf{u} due to curvature and the other independent of \mathbf{u} due to torsion, the latter associated with “closure failure” of the circuit itself. Motivated by this definition, an infinitesimal spatial Burgers vector $d\hat{\mathbf{b}}$ is, with $\mathbf{x} \rightarrow \mathbf{x} + d\hat{\mathbf{b}}$ under a Cartan displacement [14, 60],

$$d\hat{\mathbf{b}}(\mathbf{x}) = -(\hat{\mathbf{T}} + \frac{1}{2} \hat{\mathbf{R}}\mathbf{x}) : d\mathbf{a}. \quad (2.38)$$

Extending dc to a finite circuit c enclosing area a (i.e., a Burgers circuit on the deformed crystal) and choosing $\{\mathbf{g}_a\}$ constant over \mathfrak{B} , the total spatial Burgers vector is

$$\hat{\mathbf{b}} = \int_a d\hat{\mathbf{b}} = - \int_a (\hat{\mathbf{T}} + \frac{1}{2} \hat{\mathbf{R}}\mathbf{x}) : d\mathbf{a}. \quad (2.39)$$

This can be expressed in terms of defect densities using (2.33) [14]:

$$\hat{b}^a = \int_a \alpha^{ab} n_b da + \int_a d^{ac} \epsilon_{cde} \theta^{db} x^e n_b da + \int_a x^a \vartheta^b n_b da. \quad (2.40)$$

2.2 Particular cases: single defect types

It is instructive to consider cases when only one type of defect is present. A sufficient description of a crystal containing only dislocations is obtained by forcing $\mathbf{Q} = \mathbf{0}$ in (2.19), such that $\hat{\mathbf{T}} \rightarrow \bar{\mathbf{T}}$ and $\hat{\mathbf{V}} \rightarrow \bar{\mathbf{V}}$ describe a flat connection with non-vanishing torsion and vanishing nonmetricity. Differentiation of (2.12) with $d_A = \text{constant}$ yields the parallel transport equation

$$\partial_b d_a = (\partial_b F^{L-1\alpha}{}_{\alpha}) F^{Lc}{}_{\alpha} d_c = \bar{\Gamma}_{ba}^{..c} d_c \Leftrightarrow \bar{\nabla}_b d_a = 0. \quad (2.41)$$

The “local” or spatial dislocation density tensor becomes

$$\alpha = -F^L[\nabla \times (F^{L-1})], \quad \alpha^{ab} = F^{La}{}_{\alpha} \epsilon^{bcd} \partial_d F^{L-1\alpha}{}_{\alpha}. \quad (2.42)$$

Defining the “true” dislocation density and infinitesimal Burgers vector as

$$\tilde{\alpha} = F^{L-1} \alpha = -\nabla \times (F^{L-1}), \quad d\tilde{\mathbf{b}} = \tilde{\alpha} n da, \quad (2.43)$$

application of Stokes’s theorem with (2.11) produces the true Burgers vector

$$\tilde{\mathbf{b}} = \tilde{b}^a \mathbf{g}_a = \int_a d\tilde{\mathbf{b}} = \int_a \tilde{\alpha} n da = - \oint_c F^{L-1} dx = - \oint_{\mathfrak{C}} F^P dX, \quad (2.44)$$

where \mathfrak{C} is the image of c on \mathfrak{B}_0 and $\{\mathbf{g}_a\}$ are chosen constant over the domain. For a density of dislocations all having the same unit tangent line $\boldsymbol{\xi}$ and discrete Burgers vector \mathbf{b} , (2.42) yields $\alpha = \rho \mathbf{b} \otimes \boldsymbol{\xi}$, where ρ is the number of dislocations per unit area a . Accurate when ρ is not too large, in dislocation theory it is conventionally assumed

$$F^L = F^E F^I \approx F^E, \quad F = F^E F^I F^P \approx F^E F^P, \quad (2.45)$$

where F^E accounts for rigid rotation and stretch conjugate to applied stress [6, 55, 80], and F^I accounts for residual distortion (e.g., dilatation from dislocation cores) [22] not addressed by slip deformation F^P which is by definition lattice preserving [9, 10, 14, 22] and thus isochoric.

For a body containing only disclinations with no history of slip or point defects, the following conditions are imposed:

$$F = F^L = F^E F^I, \quad \alpha = 0, \quad \vartheta = 0, \quad (2.46)$$

where F^I accounts for residual deformation associated with disclinations. These lead to the following constraints that reduce \mathbf{Q} to no more than 6 independent components:

$$\bar{\Gamma}_{[bc]}^{..a} = 0, \quad \hat{T}_{bc}^{..a} = Q_{[bc]}^{..a} = 0, \quad Q_{a(bc)} = 0. \quad (2.47)$$

Thus $\hat{\Gamma}$ and $\hat{\nabla}$ now describe a Riemannian connection, i.e., vanishing torsion and nonmetricity but non-vanishing curvature. Thus a metric exists whose Levi-Civita connection is $\hat{\Gamma}$; this metric is an integral function of \mathbf{Q} that degenerates to the Levi-Civita connection of d_{ab} when \mathbf{Q} vanishes. The local Burgers vector is

$$\hat{\mathbf{b}} = \int_a d^{-1} \boldsymbol{\epsilon} : (\boldsymbol{\theta} \mathbf{n} \otimes \mathbf{x}) da. \quad (2.48)$$

For a density of disclinations all having the same unit tangent line $\boldsymbol{\xi}$ and discrete Frank rotation vector $\hat{\boldsymbol{\omega}}$, the spatial disclination density tensor is $\boldsymbol{\theta} = \rho \hat{\boldsymbol{\omega}} \otimes \boldsymbol{\xi}$, where ρ is the number of disclinations per unit area a . The infinitesimal Burgers vector then reduces to $d\hat{\mathbf{b}} = \rho d^{-1} (\hat{\boldsymbol{\omega}} \times \mathbf{x}) \langle \boldsymbol{\xi}, \mathbf{n} \rangle da$. Unlike the case for dislocations only, here the Burgers vector depends on choice of coordinate system by which \mathbf{x} is measured, i.e., $d\hat{\mathbf{b}}$ is not translationally invariant. According to (2.48), each disclination is effectively assigned a radius [14, 25, 60] measured from the origin of this coordinate system.

For a body containing only point defects, with no history of slip or disclinations, the following conditions are imposed:

$$\mathbf{F} = \mathbf{F}^L = \mathbf{F}^E \mathbf{F}^I, \quad \boldsymbol{\alpha} = \mathbf{0}, \quad \boldsymbol{\theta} = \mathbf{0}, \quad (2.49)$$

where \mathbf{F}^I accounts for residual deformation associated with point defects, which is hereafter assumed dilatational or spherical:

$$\mathbf{F}^I = (1 + \tilde{\rho} \delta v)^{1/3} \mathbf{g}_\alpha \otimes \mathbf{g}^\alpha, \quad \mathbf{F}^{I-1} = (1 - \hat{\rho} \delta v)^{-1/3} \mathbf{g}_\alpha \otimes \mathbf{g}^\alpha. \quad (2.50)$$

The number of point defects per unit reference volume is $\tilde{\rho}$, and δv is the residual volume change per defect. The number of defects per unit intermediate volume is $\hat{\rho}$, and $\hat{\rho} = \tilde{\rho} / (1 + \tilde{\rho} \delta v)$. The following constraints, necessary² for satisfaction of (2.49), are imposed, corresponding to integrable \mathbf{F}^{L-1} and vanishing (2.21) and (2.28):

$$\begin{aligned} \hat{\mathbf{T}}_{bc}^{*a} &= 0 \Rightarrow \Upsilon_{[b} \delta_{c]}^a = \frac{1}{4} d^{ad} (Q_{cbd} - Q_{cdb} - Q_{bcd} + Q_{bdc}), \\ \hat{\mathbf{R}}_{[bc][da]} &= 0 \Rightarrow 2\hat{\nabla}_{[b} Q_{c][da]} = -2Q_{[bc]}^{*e} Q_{e[da]} + Q_{b[d}^{*e} Q_{c|a]e} - Q_{c[d}^{*e} Q_{|b|a]e}. \end{aligned} \quad (2.51)$$

The local Burgers vector is

$$\hat{\mathbf{b}} = \int_a \mathbf{x} \langle \boldsymbol{\vartheta}, \mathbf{n} \rangle da. \quad (2.52)$$

As was the case for disclinations, here the Burgers vector is not translationally invariant. The Burgers vector from (2.52) is proportional to distance from the origin and is directed radially outward from the origin. If the density of point defects is uniform throughout an infinite body \mathfrak{B} , then (2.52) must vanish for any choice of coordinate system, which implies $\boldsymbol{\vartheta} = \mathbf{0}$ for any such uniform distribution.

In general, when dislocations, disclinations, and point defects are all present, three-term decomposition $\mathbf{F} = \mathbf{F}^E \mathbf{F}^I \mathbf{F}^P = \mathbf{F}^L \mathbf{F}^P$ applies. The primary distinction between \mathbf{F}^I and \mathbf{F}^P is that the former affects the lattice directors through (2.12) while the latter does not. Inelastic deformation associated with distributed disclinations and point defects includes dilatation (as well as possible shape change and rotation) and cannot be lattice-preserving; therefore, such deformation is encompassed by \mathbf{F}^I . Inelastic deformation due to dislocation glide, i.e., shearing on slip planes, is both isochoric and lattice-preserving, and is measured by \mathbf{F}^P . However, in geometrically linear theories of crystal plasticity, wherein slip directors are assumed constant, inelastic deformation from disclinations and point defects is often assigned to plastic distortion along with deformation from slip [14, 31, 32].

2.3 Nonlinear elasticity

Applications of the theory in subsequent sections consider isolated line defects (single dislocation or disclination) and isolated point defects (single vacancy or substitutional/interstitial atom). The method of solution involves assignment of a singular density of defects at a line or a point and then excluding a small region (e.g., a cylinder surrounding the line or a sphere surrounding the point) from the domain over which equilibrium equations are solved. For such applications³, the

² Previously [14, 19] conditions $Q_{a[bc]} = 0$ were imposed for a body both point defects and (possibly) dislocations; these conditions are sufficient but not necessary for vanishing disclination density.

³ In prior work [14, 25] considering time dependent problems involving continuous defect distributions, dependence of strain energy on defect densities was permitted, and additional balance laws for thermodynamic conjugates (e.g., couple stresses) to defect densities were proposed. These additional balance laws are trivially satisfied in the present context since defect densities vanish over domains excluding defect cores, but in other problems they are intended to affect kinetics and restrict equilibrium defect distributions. Proper accounting for stored energy of cold work [7] in an externally unstressed element of material requires that the element's strain energy depend on defect density [14].

following hyperelastic constitutive model for strain energy per unit reference volume W suffices:

$$W = W(\mathbf{F}^E), \quad \mathbf{P} = \partial W / \partial \mathbf{F}^E = P_a^\alpha \mathbf{g}^a \otimes \mathbf{g}_\alpha. \quad (2.53)$$

Here \mathbf{P} is a kind of (generally non-symmetric) first Piola-Kirchhoff stress. To ensure invariance under rigid rotation, it is implicitly understood that W depends only on some measure of stretch associated with \mathbf{F}^E . The usual symmetric Cauchy stress and corresponding static equilibrium equations on \mathfrak{B} , in the absence of body force, are

$$\boldsymbol{\sigma} = J^{-1} \mathbf{P} \mathbf{F}^{E\top}, \quad \nabla \cdot \boldsymbol{\sigma} = \mathbf{0}, \quad (2.54)$$

where the Jacobian determinant $J = \frac{1}{6} \epsilon_{abc} \epsilon^{ABC} F_{,A}^a F_{,B}^b F_{,C}^c = \det[\partial_A x^a] (g/G)^{1/2}$. Equilibrium equations can be mapped to the intermediate configuration $\tilde{\mathfrak{B}}$ as demonstrated in coordinate-free notation in [59, 64] and for particular choices of anholonomic coordinates in [15]; torsion of the crystal connection and possible skew-symmetric parts of the coordinate connection on \tilde{B} enter the result.

3 Screw dislocation

3.1 Geometric description

Consider a deformed body \mathfrak{B} with boundary $\partial\mathfrak{B}$. In the reference configuration, the image of this body and its boundary are \mathfrak{B}_0 and $\partial\mathfrak{B}_0$. Cylindrical coordinates covering \mathfrak{B} and \mathfrak{B}_0 are (r, θ, z) and (R, Θ, Z) and are described fully in Appendix A (See Supplementary Material, Wiley online library), including basis vectors; Cartesian coordinates are (x, y, z) and (X, Y, Z) .

An Eulerian description of deformation is invoked here, essentially inverting the Lagrangian description of Seeger and Mann [72]. Let the unit tangent line of the dislocation be oriented along the z -axis, i.e., $\boldsymbol{\xi} = \mathbf{g}_z$. The general ansatz for deformation due to a screw dislocation in an isotropic body is

$$R(r) = r - u(r), \quad \Theta(\theta) = \theta, \quad Z(\theta, z) = z - w(\varphi) - s(z). \quad (3.1)$$

Radial displacement is $u(r)$. Angle θ is multi-valued upon complete revolutions around the dislocation line. Slip plane \mathfrak{S} corresponds to the half-plane ($y = 0, x < 0$), or $\theta = \pm\pi$. Following [32], φ is introduced to maintain uniqueness of the deformation field and enable description of the slip discontinuity via generalized functional analysis [39]. Angle φ is single valued but discontinuous, and is defined as [32]

$$\varphi(x, y) = \tan^{-1}(y/x) + \pi \mathbf{H}(-x)[\mathbf{H}(y) - \mathbf{H}(-y)], \quad (3.2)$$

where the arctangent is restricted to its principal value in the range $(-\frac{\pi}{2}, \frac{\pi}{2})$ and

$$\mathbf{H}(x) = 0 \quad \forall x < 0; \quad \mathbf{H}(x) = 1 \quad \forall x > 0. \quad (3.3)$$

Note that

$$\varphi \in (-\pi, \pi), \quad \llbracket \varphi \rrbracket = \varphi|_{\theta=\pi} - \varphi|_{\theta=-\pi} = 2\pi, \quad \varphi = \theta \quad \forall \theta \in (-\pi, \pi). \quad (3.4)$$

Generalized derivatives [39] of $\varphi(x, y)$ are [32]:

$$\partial_x \varphi = -y/r^2, \quad \partial_y \varphi = x/r^2 + 2\pi \mathbf{H}(-x) \delta(y), \quad (3.5)$$

where $\delta(y) = d\mathbf{H}(y)/dy = \mathbf{H}'(y)$ is the Dirac delta function. The following generalized derivatives are also noted for functions whose ordinary derivatives are $\mathcal{O}(1/r^2)$ [32]:

$$\partial_x (x/r^2) = 1/r^2 - 2x^2/r^4 + \pi \delta(r), \quad \partial_y (y/r^2) = 1/r^2 - 2y^2/r^4 + \pi \delta(r), \quad (3.6)$$

where $\delta(r) = \delta(x)\delta(y)$ in polar cylindrical coordinates.

For the screw dislocation, the true Burgers vector and function w are

$$\tilde{\mathbf{b}} = \tilde{b} \mathbf{g}_z = \tilde{b} \mathbf{G}_Z, \quad w = \tilde{b} \varphi / (2\pi). \quad (3.7)$$

The true Burgers vector is constant. Since $\theta = \Theta$, basis vectors in Appendix A (See Supplementary Material, Wiley online library) here obey $(1/r) \mathbf{g}_\theta = (1/R) \mathbf{G}_\Theta = \mathbf{e}_\theta = \mathbf{E}_\Theta$. Displacement $\mathbf{u} = \mathbf{x} - \mathbf{X}$ in (A.38) reduces to

$$\mathbf{u} = u(r) \mathbf{g}_r + [w(\varphi) + s(z)] \mathbf{g}_z = u(r) \mathbf{G}_R + [w(\varphi) + s(z)] \mathbf{G}_Z. \quad (3.8)$$

Displacement is continuous except for that due to the jump in w across \mathfrak{S} :

$$[\mathbf{u}] = \mathbf{u}|_{\theta=\pi} - \mathbf{u}|_{\theta=-\pi} = \tilde{\mathbf{b}}. \quad (3.9)$$

In curvilinear coordinates, the inverse deformation gradient from (3.1) is

$$\begin{aligned} \mathbf{F}^{-1} &= F^{-1R}_{,r} \mathbf{G}_R \otimes \mathbf{g}^r + F^{-1\Theta}_{,\theta} \mathbf{G}_\Theta \otimes \mathbf{g}^\theta + F^{-1Z}_{,z} \mathbf{G}_Z \otimes \mathbf{g}^z + F^{-1}_{,\theta} \mathbf{G}_Z \otimes \mathbf{g}^\theta \\ &= (\mathrm{d}R/\mathrm{d}r) \mathbf{G}_R \otimes \mathbf{g}^r + \mathbf{G}_\Theta \otimes \mathbf{g}^\theta + \partial_z Z \mathbf{G}_Z \otimes \mathbf{g}^z + \partial_\theta Z \mathbf{G}_Z \otimes \mathbf{g}^\theta \\ &= [1 - u'(r)] \mathbf{G}_R \otimes \mathbf{g}^r + \mathbf{G}_\Theta \otimes \mathbf{g}^\theta + [1 - s'(z)] \mathbf{G}_Z \otimes \mathbf{g}^z - \partial_\theta w \mathbf{G}_Z \otimes \mathbf{g}^\theta, \end{aligned} \quad (3.10)$$

where $u' = \mathrm{d}u/\mathrm{d}r$ and $s' = \mathrm{d}s/\mathrm{d}z$. From (3.5),

$$F^{-1Z}_{,\theta} = -\frac{\tilde{b}}{2\pi} [-r \sin \theta \partial_x w + r \cos \theta \partial_y w] = -\frac{\tilde{b}}{2\pi} [1 - 2\pi r H(-x) \delta(y)]. \quad (3.11)$$

To fix translational invariance of the origin and ensure volume remains positive,

$$u(0) = 0, \quad s(0) = 0; \quad (1 - u/r)(1 - u')(1 - s') > 0. \quad (3.12)$$

The final decomposition (2.45) is now applied, such that

$$\mathbf{F} = \mathbf{F}^E \mathbf{F}^P, \quad \mathbf{F}^{-1} = \mathbf{F}^{P-1} \mathbf{F}^{E-1}. \quad (3.13)$$

Extending the linear theory of De Wit [32] to the geometrically nonlinear regime, the “elastic” part of \mathbf{F}^{-1} is defined as that which is continuous and single-valued over \mathfrak{B} except at $r = 0$:

$$\mathbf{F}^{E-1} = [1 - u'(r)] \mathbf{G}_R \otimes \mathbf{g}^r + \mathbf{G}_\Theta \otimes \mathbf{g}^\theta + [1 - s'(z)] \mathbf{G}_Z \otimes \mathbf{g}^z - [\tilde{b}/(2\pi)] \mathbf{G}_Z \otimes \mathbf{g}^\theta. \quad (3.14)$$

It follows from (3.11) and (3.13) that

$$\mathbf{F}^{-1} = \tilde{b}r H(-x) \delta(y) \mathbf{G}_Z \otimes \mathbf{g}^\theta + \mathbf{F}^{E-1} = [\tilde{b}r H(-x) \delta(y) \mathbf{G}_Z \otimes (\mathbf{F}^{E\top} \mathbf{g}^\theta) + \mathbf{1}] \mathbf{F}^{E-1}. \quad (3.15)$$

In the reference configuration, the image of the slipped surface \mathfrak{S}_0 is $(X < 0, Y = 0)$, on which $r(R)$ and $\theta(\Theta)$ are continuous, but $Z(\theta, z)$ is discontinuous. Let \mathbf{m} denote a normal to \mathfrak{S} directed from $\Theta = -\pi$ to $\Theta = +\pi$:

$$\mathbf{m}(r, R) = -r \mathbf{g}^\theta \cdot \mathbf{F}^E = -r \mathbf{G}^\Theta = -(1/R) \mathbf{g}_\theta = -(r/R) \mathbf{e}_\theta \quad \text{on } \mathfrak{S}. \quad (3.16)$$

The plastic part of (3.15) is the simple shear

$$\mathbf{F}^{P-1}(\mathbf{x}) = \mathbf{1} - H(-x) \delta(y) \tilde{\mathbf{b}} \otimes \mathbf{m}, \quad \mathbf{F}^P(\mathbf{X}) = \mathbf{1} + H(-X) \delta(Y) \tilde{\mathbf{b}} \otimes \mathbf{m}. \quad (3.17)$$

Since $\tilde{\mathbf{b}} \cdot \mathbf{m} = -(\tilde{b}r/R) \mathbf{e}_z \cdot \mathbf{e}_\theta = 0$, slip is isochoric: $\det \mathbf{F}^P = 1$. Integration of \mathbf{F}^P over a rectangular volume V traversed by \mathfrak{S}_0 produces, with the approximation $r/R \approx 1$,

$$(1/V) \int_V \mathbf{F}^P \mathrm{d}V \approx \mathbf{1} + V^{-1} \tilde{\mathbf{b}} \otimes \mathbf{m} \int_V H(-X) \delta(Y) \mathrm{d}X \mathrm{d}Y \mathrm{d}Z = \mathbf{1} + \gamma \mathbf{s} \otimes \mathbf{m}, \quad (3.18)$$

where $\gamma = \tilde{b}A/V$ is shear in direction $\mathbf{s} = \mathbf{g}_z$ due to slip over area $A = \int H(-X) \mathrm{d}X \mathrm{d}Z$. From the above description,

$$\begin{aligned} \mathbf{F}(\mathbf{X}) &= \mathbf{F}^E \quad \forall \mathbf{X} \in \mathfrak{B}_0 \setminus \mathfrak{S}_0, & \mathbf{F}(\mathbf{X}) &= \mathbf{F}^E \mathbf{F}^P \quad \text{on } \mathfrak{S}_0; \\ \mathbf{F}^{-1}(\mathbf{x}) &= \mathbf{F}^{E-1} \quad \forall \mathbf{x} \in \mathfrak{B} \setminus \mathfrak{S}, & \mathbf{F}^{-1}(\mathbf{x}) &= \mathbf{F}^{P-1} \mathbf{F}^{E-1} \quad \text{on } \mathfrak{S}. \end{aligned} \quad (3.19)$$

It becomes prudent to select coincident cylindrical coordinate systems on $\tilde{\mathfrak{B}}$ and \mathfrak{B}_0 , such that $\mathbf{g}_\alpha(\mathbf{X}) = \delta_\alpha^A \mathbf{G}_A(\mathbf{X})$ [15], and in these coordinates

$$\mathbf{F}^E = F^{E\ a}_{,\alpha} \mathbf{g}_a \otimes \mathbf{g}^\alpha = F^{E\ a}_{,A} \mathbf{g}_a \otimes \mathbf{G}^A, \quad F^{E\ a}_{,A}(\mathbf{X}) = \partial_A x^a(\mathbf{X}) \quad \forall \mathbf{X} \in \mathfrak{B}_0 \setminus \mathfrak{S}_0. \quad (3.20)$$

The dislocation density tensor can now be computed. In Cartesian coordinates, using (3.5),

$$F^{-1Z}_{,x} = \tilde{b}y/(2\pi r^2), \quad F^{-1Z}_{,y} = -\tilde{b}[x/(2\pi r^2) + H(-x) \delta(y)]. \quad (3.21)$$

Decomposing this into continuous and singular parts,

$$F^{E-1Z}_{,x} = \tilde{b}y/(2\pi r^2), \quad F^{E-1Z}_{,y} = -\tilde{b}x/(2\pi r^2), \quad F^{P-1Z}_{,y} = -\tilde{b}H(-x)\delta(y). \quad (3.22)$$

The only non-vanishing component of true dislocation density is, from (2.43) and (3.6),

$$\tilde{\alpha}^{Zz} = \epsilon^{zbc} \partial_c F^{E-1Z}_{,b} = \partial_y F^{E-1Z}_{,x} - \partial_x F^{E-1Z}_{,y} = [\tilde{b}/(2\pi)][\partial_y(y/r^2) + \partial_x(x/r^2)] = \tilde{b}\delta(r). \quad (3.23)$$

Therefore,

$$\tilde{\alpha} = \tilde{b}\delta(r)G_Z \otimes g_z = \delta(r)\tilde{b} \otimes \xi. \quad (3.24)$$

Consider a closed loop \mathfrak{c} encircling the dislocation line; area a enclosed by this loop has constant normal vector $\mathbf{n} = g_z = \xi$. Applying Stokes's theorem, consistency with (2.44) with $\mathbf{F}^E = \mathbf{F}^L$ is demonstrated:

$$\begin{aligned} \tilde{b} &= \int_a \delta(r)\tilde{b}\langle \xi, \mathbf{n} \rangle r dr d\theta = - \int_a (\nabla \times \mathbf{F}^{E-1}) \mathbf{n} da \\ &= - \oint_{\mathfrak{c}} \mathbf{F}^{E-1} d\mathbf{x} = - \oint_{\mathfrak{c}} F^{E-1Z}_{,\theta} G_Z d\theta = \frac{\tilde{b}}{2\pi} \oint_{\mathfrak{c}} d\theta = \tilde{b}. \end{aligned} \quad (3.25)$$

The second of (2.9) can be verified by taking the curl, in the sense of a generalized derivative [39], of (3.15):

$$-\nabla \times (\mathbf{F}^{-1}) = -\nabla \times (\mathbf{F}^{E-1}) + \nabla \times [H(-x)\delta(y)\tilde{b} \otimes \mathbf{m}] = \tilde{\alpha} - \delta(-x)\delta(y)\tilde{b} \otimes g_z = \mathbf{0}. \quad (3.26)$$

3.2 Nonlinear elastic analysis and general solution

A nonlinear elastic boundary value problem for the screw dislocation is constructed as follows. Let body \mathfrak{B} consist of a cylinder of outer radius R_0 with the dislocation line located along $r = 0$. A cylindrical core region $r < r_0$ is removed from the body and excluded from the solution domain. The length of the cylinder is L , such that the body is contained within the limits $-\frac{L}{2} \leq z \leq \frac{L}{2}$, though the forthcoming analysis also applies for the case $L \rightarrow \infty$. Slip plane \mathfrak{S} now consists of the two-sided flat region ($\theta = \pm\pi, r_0 < r < R_0$). Body \mathfrak{B} is multiply connected when it contains the slip plane (i.e., when it is treated as an annular tube) since θ is multi-valued. Domain $\mathfrak{B} \setminus \mathfrak{S}$ is simply connected, as is its image in the reference configuration $\mathfrak{B}_0 \setminus \mathfrak{S}_0$.

Equilibrium equations are solved on $\mathfrak{B} \setminus \mathfrak{S}$. From (3.19), in this domain the strain energy function in (2.53) becomes

$$W = W(\mathbf{F}) = \hat{W}[\mathbf{D}(\mathbf{F})] = \bar{W}[\mathbf{E}(\mathbf{F})]. \quad (3.27)$$

As defined in Appendix C (See Supplementary Material, Wiley online library), Eulerian and Lagrangian strain measures (both referred to material coordinates $\{X^A\}$) are, respectively,

$$\mathbf{D} = \frac{1}{2}(\mathbf{1} - \mathbf{F}^{-1}\mathbf{F}^{-T}), \quad \mathbf{E} = \frac{1}{2}(\mathbf{F}^T\mathbf{F} - \mathbf{1}). \quad (3.28)$$

Cauchy stress is, from (C.6),

$$\boldsymbol{\sigma} = J^{-1}\mathbf{P}\mathbf{F}^T = J^{-1}\mathbf{F}^{-T}\hat{\mathbf{S}}\mathbf{F}^{-1} = J^{-1}\mathbf{F}\bar{\mathbf{S}}\mathbf{F}^T, \quad (3.29)$$

where

$$\mathbf{P} = \partial W / \partial \mathbf{F}, \quad \hat{\mathbf{S}} = \partial \hat{W} / \partial \mathbf{D}, \quad \bar{\mathbf{S}} = \partial \bar{W} / \partial \mathbf{E}. \quad (3.30)$$

Static equilibrium equations are

$$\nabla \cdot \boldsymbol{\sigma} = \mathbf{0}, \quad \nabla_b \sigma^{ab} = 0. \quad (3.31)$$

Internal boundary conditions are

$$[\mathbf{u}] = \tilde{b} \quad \text{on} \quad \mathfrak{S}; \quad \mathbf{t}|_{r=r_0} = \boldsymbol{\sigma}\mathbf{n} = \tilde{p}\mathbf{e}_r \Rightarrow \sigma^{rr}|_{r=r_0} = -\tilde{p}. \quad (3.32)$$

The first of (3.32) prescribes a displacement jump equal to the true Burgers vector across the slip plane, as in (3.9). The second of (3.32) assigns a traction \mathbf{t} at the core surface corresponding to a constant radial Cauchy pressure \tilde{p} , with \mathbf{e}_r a unit

vector in the radial direction as defined in Appendix A (See Supplementary Material, Wiley online library). Traction along the core must be a uniform pressure to maintain consistency with the symmetry inherent in ansatz (3.1). External boundary conditions are

$$t|_{r=R_0} = \mathbf{0}; \quad \left(\int_{r_0}^{R_0} t^z r dr d\theta \right) \Big|_{z=\pm L/2} = 0 \quad \text{or} \quad s(z) \rightarrow 0 \quad \text{as} \quad L \rightarrow \infty. \quad (3.33)$$

The first of (3.33) prescribes traction free conditions on the surface of the cylinder at $r = R_0$. The second of (3.33) prescribes either null average axial force for a cylinder of finite length, or no average axial strain for an infinite cylinder.

An iterative solution procedure in Eulerian coordinates is invoked, similar to that of Teodosiu and S6os [81, 82]. The primary difference between the present isotropic nonlinear elastic analysis of the screw dislocation and that in [81] is that here a different (Eulerian) strain energy potential \hat{W} is used, in contrast to the Lagrangian strain energy potential \bar{W} used in [81, 82]. A second difference is that possible axial strains are considered for a dislocation of finite length, in contrast to [81] that considered only the infinitely long dislocation and imposed $s = 0$. In an earlier analysis of the screw dislocation in isotropic nonlinear elasticity, Seeger and Mann [72] used an iterative procedure in Lagrangian coordinates, with a Lagrangian strain energy function, and allowed for axial strain, but did not address core pressure. The general method of solution in Lagrangian coordinates was described formally by Gairola [38].

According to the method of solution [81, 82], spatial displacement \mathbf{u} is written in the series

$$\mathbf{u}(\mathbf{x}) = k\mathbf{u}_0(\mathbf{x}) + k^2\mathbf{u}_1(\mathbf{x}) + \cdots, \quad (3.34)$$

where $k > 0$ is a small scalar parameter whose particular value will not affect the final solution. Internal boundary conditions are of the assumed form

$$\tilde{\mathbf{b}} = k\mathbf{b}, \quad \tilde{p} = kp, \quad (3.35)$$

which is justified by the vanishing of $\tilde{\mathbf{b}}$ with \tilde{p} [81, 82]. Truncating (3.34) at second order⁴ [i.e., omitting terms of $O(k^3)$] and prescribing a strain energy potential of either of the latter two forms in (3.27) results in a series expression for Cauchy stress:

$$\boldsymbol{\sigma} = k\boldsymbol{\sigma}_0 + k^2(\boldsymbol{\sigma}_1 + \boldsymbol{\tau}), \quad \sigma_0^{ab} = C^{abcd}\nabla_c(u_0)_d, \quad \sigma_1^{ab} = C^{abcd}\nabla_c(u_1)_d, \quad (3.36)$$

where C^{abcd} are second-order elastic constants (equivalent to those introduced in Appendix C (See Supplementary Material, Wiley online library)), and where $\boldsymbol{\tau}$ depends on $\nabla\mathbf{u}_0$ and second- and third-order elastic constants. Substituting into (3.31), two sets of equilibrium equations result:

$$\nabla \cdot \boldsymbol{\sigma}_0 = \mathbf{0}, \quad \nabla \cdot \boldsymbol{\sigma}_1 = -\nabla \cdot \boldsymbol{\tau}. \quad (3.37)$$

The first of these equations is solved in conjunction with internal boundary conditions linear in k , i.e., (3.35), providing a solution for \mathbf{u}_0 . The second of these equations is then solved for \mathbf{u}_1 , applying continuity of \mathbf{u}_1 across \mathfrak{S} and null traction at $r = r_0$, along with the previously obtained solution for \mathbf{u}_0 to be used to compute $\boldsymbol{\tau}$. For both solutions, vanishing traction at $r = R_0$ is imposed.

The general method of solution is now applied to the screw dislocation, where $\hat{W}(\mathbf{D})$ is used for the strain energy potential, making the present analysis and results different from others mentioned already [38, 72, 81]. Displacement (3.34) applied to (3.8) results in

$$u(r) = ku_0(r) + k^2u_1(r), \quad w(\varphi) = kw_0(\varphi) = kb\varphi/(2\pi), \quad s(z) = ks_0(z) + k^2s_1(z), \quad (3.38)$$

where w is necessarily truncated at first order to satisfy (3.7) and (3.35), with

$$\tilde{\mathbf{b}} = kb\mathbf{G}_Z, \quad \tilde{b} = kb. \quad (3.39)$$

With respect to curvilinear cylindrical bases $\{\mathbf{G}_A, \mathbf{g}^a\}$, the inverse deformation gradient matrix on $\mathfrak{B} \setminus \mathfrak{S}$ is

$$[F^{-1A}_{\cdot a}] = \begin{bmatrix} R' & 0 & 0 \\ 0 & \Theta' & 0 \\ 0 & \partial_\theta Z & \partial_z Z \end{bmatrix} = \begin{bmatrix} 1 - ku'_0 - k^2u'_1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -kb/(2\pi) & 1 - ks'_0 - k^2s'_1 \end{bmatrix}. \quad (3.40)$$

⁴ Incorporation of terms cubic in k would result in a problem depending on fourth-order elastic constants, which cannot be measured completely, and are usually unknown for real crystals.

As remarked already, the domain of analysis excludes the core and slip plane and thereby avoids singularities and consideration of \mathbf{F}^P . In physical components, i.e., orthonormal bases $\{\mathbf{e}_a, \mathbf{E}_A\}$, (A.36) becomes, for the isolated screw dislocation,

$$[F^{-1}]_{\langle Aa \rangle} = \begin{bmatrix} 1 - ku'_0 - k^2 u'_1 & 0 & 0 \\ 0 & 1 - ku_0/r - k^2 u_1/r & 0 \\ 0 & -kb/(2\pi r) & 1 - ks'_0 - k^2 s'_1 \end{bmatrix}, \quad (3.41)$$

noting that $\sqrt{G/g} = R/r = 1 - u/r$. Henceforth, such physical components will be used for analysis of the screw dislocation. Volume ratio is

$$\begin{aligned} J^{-1} &= \det[F^{-1}]_{\langle Aa \rangle} = (1 - ku'_0 - k^2 u'_1)(1 - ku_0/r - k^2 u_1/r)(1 - ks'_0 - k^2 s'_1) \\ &= 1 - k(u'_0 + u_0/r + s'_0) + O(k^2). \end{aligned} \quad (3.42)$$

The next step is computation of components of strain tensor \mathbf{D} in terms of the quantities $(k, b, u', u/r, s')$. Subsequent algebra becomes analytically intractable when all such quantities are retained in the general solution. Therefore, two particular cases are considered in what follows:

$$p = 0 \Rightarrow s_0 = 0; \quad \text{or} \quad L \rightarrow \infty \Rightarrow s = 0. \quad (3.43)$$

The first case is consistent with a priori knowledge that in the linear elastic solution of a screw dislocation, axial strain vanishes when core pressure vanishes⁵. This is the Eulerian analog of the form of Lagrangian displacement function $s(Z)$ assumed by Seeger and Mann [72]. The second case in (3.43) is consistent with the second set of boundary conditions in (3.33), and leads to the condition that all displacements are independent of z , as should be the case for an infinitely long dislocation line. Therefore,

$$s(z) = k^2 s_1(z) \quad (3.44)$$

is used, with $s_1 = 0$ invoked when boundary conditions corresponding to the second case are imposed.

In physical cylindrical components, strain tensor \mathbf{D} is, from (3.28) and (3.41),

$$\mathbf{D} = D_{RR} \mathbf{E}_R \otimes \mathbf{E}_R + D_{\Theta\Theta} \mathbf{E}_\Theta \otimes \mathbf{E}_\Theta + D_{ZZ} \mathbf{E}_Z \otimes \mathbf{E}_Z + D_{\Theta Z} (\mathbf{E}_\Theta \otimes \mathbf{E}_Z + \mathbf{E}_Z \otimes \mathbf{E}_\Theta); \quad (3.45)$$

$$\begin{aligned} D_{RR} &= ku'_0 + k^2(u'_1 - \tfrac{1}{2}u_0'^2), & D_{\Theta\Theta} &= ku_0/r + k^2[u_1/r - \tfrac{1}{2}(u_0/r)^2], \\ D_{ZZ} &= k^2[s'_1 - b^2/(8\pi^2 r^2)], & D_{\Theta Z} &= D_{Z\Theta} = kb/(4\pi r) - k^2 bu_0/(4\pi r^2), \end{aligned} \quad (3.46)$$

where terms $O(k^3)$ have been truncated. Strain energy potential per unit reference volume (C.7) is used, truncated at third order:

$$\begin{aligned} \hat{W} &= \tfrac{1}{2} C_{ABCD} D_{AB} D_{CD} + \tfrac{1}{6} \hat{C}_{ABCDEF} D_{AB} D_{CD} D_{EF} \\ &= \tfrac{1}{2} C_{\alpha\beta} D_\alpha D_\beta + \tfrac{1}{6} \hat{C}_{\alpha\beta\gamma} D_\alpha D_\beta D_\gamma, \end{aligned} \quad (3.47)$$

where Greek subscripts denote Voigt notation. For an isotropic material, second-order constants $C_{\alpha\beta}$ depend on (λ, μ) from (C.11), and third-order constants $\hat{C}_{\alpha\beta\gamma}$ depend on $(\hat{\nu}_1, \hat{\nu}_2, \hat{\nu}_3)$ from (C.12). Stress $\hat{\mathbf{S}} = \partial \hat{W} / \partial \mathbf{D}$ is, omitting terms of $O(k^3)$,

$$\hat{\mathbf{S}} = \hat{S}_{RR} \mathbf{E}_R \otimes \mathbf{E}_R + \hat{S}_{\Theta\Theta} \mathbf{E}_\Theta \otimes \mathbf{E}_\Theta + \hat{S}_{ZZ} \mathbf{E}_Z \otimes \mathbf{E}_Z + \hat{S}_{\Theta Z} (\mathbf{E}_\Theta \otimes \mathbf{E}_Z + \mathbf{E}_Z \otimes \mathbf{E}_\Theta); \quad (3.48)$$

$$\begin{aligned} \hat{S}_{RR} &= k\{(\lambda + 2\mu)u'_0 + \lambda u_0/r\} \\ &\quad + k^2\{(\lambda + 2\mu)(u'_1 - u_0'^2/2) + \lambda[u_1/r - \tfrac{1}{2}(u_0/r)^2 + s'_1 - b^2/(8\pi^2 r^2)] \\ &\quad + \tfrac{1}{2}(\hat{\nu}_1 + 6\hat{\nu}_2 + 8\hat{\nu}_3)u_0'^2 + (\hat{\nu}_1 + 2\hat{\nu}_2)[\tfrac{1}{2}(u_0/r)^2 + u'_0 u_0/r] + \hat{\nu}_2 b^2/(8\pi^2 r^2)\}, \end{aligned} \quad (3.49)$$

$$\begin{aligned} \hat{S}_{\Theta\Theta} &= k\{(\lambda + 2\mu)u_0/r + \lambda u'_0\} \\ &\quad + k^2\{(\lambda + 2\mu)[u_1/r - \tfrac{1}{2}(u_0/r)^2] + \lambda[u'_1 - u_0'^2/2 + s'_1 - b^2/(8\pi^2 r^2)] \\ &\quad + \tfrac{1}{2}(\hat{\nu}_1 + 6\hat{\nu}_2 + 8\hat{\nu}_3)(u_0/r)^2 + (\hat{\nu}_1 + 2\hat{\nu}_2)(u_0'^2/2 + u'_0 u_0/r) \\ &\quad + (\hat{\nu}_2 + 2\hat{\nu}_3)b^2/(8\pi^2 r^2)\}, \end{aligned} \quad (3.50)$$

⁵ It will be shown explicitly later how positive core pressure p is linearly proportional to axial contraction in the linear solution.

$$\begin{aligned}\hat{S}_{ZZ} &= k\{\lambda(u'_0 + u_0/r)\} \\ &\quad + k^2\{(\lambda + 2\mu)[s'_1 - b^2/(8\pi^2 r^2)] + \lambda[u'_1 + u_1/r - u_0'^2/2 - \frac{1}{2}(u_0/r)^2] \\ &\quad + \frac{1}{2}(\hat{\nu}_1 + 2\hat{\nu}_2)[u_0'^2 + (u_0/r)^2] + \hat{\nu}_1 u'_0 u_0/r + (\hat{\nu}_2 + 2\hat{\nu}_3)b^2/(8\pi^2 r^2)\},\end{aligned}\quad (3.51)$$

$$\hat{S}_{\Theta Z} = \hat{S}_{Z\Theta} = k\{\mu b/(2\pi r)\} - k^2\{\mu b u_0/(2\pi r^2)\}.\quad (3.52)$$

Using (3.41) and (3.42), Cauchy stress $\boldsymbol{\sigma} = J^{-1} \mathbf{F}^{-T} \hat{\mathbf{S}} \mathbf{F}^{-1}$ is, omitting terms of $O(k^3)$,

$$\boldsymbol{\sigma} = \sigma_{rr} \mathbf{e}_r \otimes \mathbf{e}_r + \sigma_{\theta\theta} \mathbf{e}_\theta \otimes \mathbf{e}_\theta + \sigma_{zz} \mathbf{e}_z \otimes \mathbf{e}_z + \sigma_{\theta z} (\mathbf{e}_\theta \otimes \mathbf{e}_z + \mathbf{e}_z \otimes \mathbf{e}_\theta);\quad (3.53)$$

$$\begin{aligned}\sigma_{rr} &= k\{(\lambda + 2\mu)u'_0 + \lambda u_0/r\} \\ &\quad + k^2\{(\lambda + 2\mu)u'_1 + \lambda(u_1/r + s'_1) - \frac{1}{2}(7\lambda + 14\mu - \hat{\nu}_1 - 6\hat{\nu}_2 - 8\hat{\nu}_3)u_0'^2 \\ &\quad - (4\lambda + 2\mu - \hat{\nu}_1 - 2\hat{\nu}_2)u'_0 u_0/r - \frac{1}{2}(3\lambda - \hat{\nu}_1 - 2\hat{\nu}_2)(u_0/r)^2 \\ &\quad - (\lambda - \hat{\nu}_2)b^2/(8\pi^2 r^2)\},\end{aligned}\quad (3.54)$$

$$\begin{aligned}\sigma_{\theta\theta} &= k\{(\lambda + 2\mu)u_0/r + \lambda u'_0\} \\ &\quad + k^2\{(\lambda + 2\mu)u_1/r + \lambda(u'_1 + s'_1) - \frac{1}{2}(3\lambda - \hat{\nu}_1 - 2\hat{\nu}_2)u_0'^2 \\ &\quad - (4\lambda + 2\mu - \hat{\nu}_1 - 2\hat{\nu}_2)u'_0 u_0/r - \frac{1}{2}(7\lambda + 14\mu - \hat{\nu}_1 - 6\hat{\nu}_2 - 8\hat{\nu}_3)(u_0/r)^2 \\ &\quad - (\lambda + 2\mu - \hat{\nu}_2 - 2\hat{\nu}_3)b^2/(8\pi^2 r^2)\},\end{aligned}\quad (3.55)$$

$$\begin{aligned}\sigma_{zz} &= k\{\lambda(u'_0 + u_0/r)\} \\ &\quad + k^2\{\lambda(u'_1 + u_1/r) + (\lambda + 2\mu)s'_1 - \frac{1}{2}(3\lambda - \hat{\nu}_1 - 2\hat{\nu}_2)u_0'^2 \\ &\quad - (2\lambda - \hat{\nu}_1)u'_0 u_0/r - \frac{1}{2}(3\lambda - \hat{\nu}_1 - 2\hat{\nu}_2)(u_0/r)^2 \\ &\quad - (\lambda + 4\mu - \hat{\nu}_2 - 2\hat{\nu}_3)b^2/(8\pi^2 r^2)\},\end{aligned}\quad (3.56)$$

$$\sigma_{\theta z} = \sigma_{z\theta} = k\{\mu b/(2\pi r)\} - k^2\{(\lambda + \mu)bu'_0/(2\pi r) + (\lambda + 4\mu)bu_0/(2\pi r^2)\}.\quad (3.57)$$

These are consistent with (3.36). From symmetry of Cauchy stress, applying (A.39) in spatial components, equilibrium equations $\nabla \cdot \boldsymbol{\sigma} = \mathbf{0}$ reduce to

$$\partial_r \sigma_{rr} + (\sigma_{rr} - \sigma_{\theta\theta})/r = 0, \quad \partial_\theta \sigma_{\theta\theta}/r + \partial_z \sigma_{\theta z} = 0, \quad \partial_\theta \sigma_{\theta z}/r + \partial_z \sigma_{zz} = 0.\quad (3.58)$$

First consider equilibrium conditions corresponding to stress components linear in k , i.e., the first of (3.37), where

$$\begin{aligned}\boldsymbol{\sigma}_0(r) &= [(\lambda + 2\mu)u'_0 + \lambda u_0/r] \mathbf{e}_r \otimes \mathbf{e}_r + [(\lambda + 2\mu)u_0/r + \lambda u'_0] \mathbf{e}_\theta \otimes \mathbf{e}_\theta \\ &\quad + [\lambda(u'_0 + u_0/r)] \mathbf{e}_z \otimes \mathbf{e}_z + [\mu b/(2\pi r)] (\mathbf{e}_\theta \otimes \mathbf{e}_z + \mathbf{e}_z \otimes \mathbf{e}_\theta).\end{aligned}\quad (3.59)$$

Since $\boldsymbol{\sigma}_0$ does not depend on θ or z , the second and third equilibrium equations in (3.58) are trivially satisfied to first order in k . The first order radial equilibrium equation becomes

$$(\lambda + 2\mu)(u_0'' + \lambda u'_0/r - u_0/r^2) = 0.\quad (3.60)$$

This is a homogeneous second-order ordinary differential equation of Cauchy-Euler type, with general solution

$$u_0 = c_1 r + c_2/r.\quad (3.61)$$

Applying boundary conditions $(\sigma_0)_{rr}|_{r=r_0} = -p$ and $(\sigma_0)_{rr}|_{r=R_0} = 0$, the solution is

$$c_1 = \chi(1 - 2\nu), \quad c_2 = \chi R_0^2, \quad \chi = [p/(2\mu)][r_0^2/(R_0^2 - r_0^2)],\quad (3.62)$$

with Poisson's ratio ν defined in (C.14). With u_0 now known, all components of σ_0 can be found using (3.59). To first order in k , radial displacement, radial stress, circumferential stress, and axial stress vanish if core pressure is omitted ($\chi = 0$), whereby the solution degenerates to the usual anti-plane shear description of a screw dislocation in isotropic linear elasticity. It was assumed in (3.44) that $s_0(z) = 0$. If this restriction is relaxed in the linear solution, then the axial equilibrium equation yields $(\lambda + 2\mu)s_0'' = 0 \Rightarrow s_0 = c_3 z$. If the average axial stress $(\sigma_0)_{zz}$ is set to zero over any cross section of the cylinder at constant z , then $s_0 = -2[\nu(1 - 2\nu)/(1 - \nu)]\chi z$ is the axial contraction that occurs in conjunction with positive core pressure for $\nu > 0$. Since $s_0 = 0$ when $\chi = 0$, the first assumption in (3.43) is now verified.

Now consider equilibrium equations for stress components quadratic in k , i.e., the second of (3.37). From (3.54)–(3.57),

$$\begin{aligned} \sigma_1(r, z) = & [(\lambda + 2\mu)u_1' + \lambda(u_1/r + s_1')]e_r \otimes e_r + [(\lambda + 2\mu)u_1/r + \lambda(u_1' + s_1')]e_\theta \otimes e_\theta \\ & + [(\lambda + 2\mu)s_1' + \lambda(u_1' + u_1/r)]e_z \otimes e_z, \end{aligned} \quad (3.63)$$

$$\begin{aligned} \tau(r) = & \{\chi^2(1 - 2\nu)^2(-9\lambda - 9\mu + 2\hat{\nu}_1 + 6\hat{\nu}_2 + 4\hat{\nu}_3) \\ & + (1/r^2)[\chi^2 R_0^2(1 - 2\nu)(4\lambda + 14\mu - 4\hat{\nu}_2 - 8\hat{\nu}_3) - (\lambda - \hat{\nu}_2)b^2/(8\pi^2)] \\ & + (1/r^4)[\chi^2 R_0^4(-\lambda - 5\mu + 2\hat{\nu}_2 + 4\hat{\nu}_3)]\}e_r \otimes e_r \\ & + \{\chi^2(1 - 2\nu)^2(-9\lambda - 9\mu + 2\hat{\nu}_1 + 6\hat{\nu}_2 + 4\hat{\nu}_3) \\ & + (1/r^2)[\chi^2 R_0^2(1 - 2\nu)(-4\lambda - 14\mu + 4\hat{\nu}_2 + 8\hat{\nu}_3) \\ & - (\lambda + 2\mu - \hat{\nu}_2 - 2\hat{\nu}_3)b^2/(8\pi^2)] \\ & + (1/r^4)[\chi^2 R_0^4(-\lambda - 5\mu + 2\hat{\nu}_2 + 4\hat{\nu}_3)]\}e_\theta \otimes e_\theta \\ & + \{\chi^2(1 - 2\nu)^2(-5\lambda + 2\hat{\nu}_1 + 2\hat{\nu}_2) + (1/r^2)[(-\lambda - 4\mu + \hat{\nu}_2 + 2\hat{\nu}_3)b^2/(8\pi^2)] \\ & + (1/r^4)[\chi^2 R_0^4(-\lambda + 2\hat{\nu}_2)]\}e_z \otimes e_z \\ & - \{(1/r)[(1 - 2\nu)(2\lambda + 5\mu)b\chi/(2\pi)] \\ & + (1/r^3)[3\mu b\chi R_0^2/(2\pi)]\}(e_\theta \otimes e_z + e_z \otimes e_\theta). \end{aligned} \quad (3.64)$$

The radial component of second-order equilibrium equation in (3.37) is

$$\partial_r(\sigma_1 + \tau)_{rr} + [(\sigma_1 + \tau)_{rr} - (\sigma_1 + \tau)_{\theta\theta}]/r = 0. \quad (3.65)$$

Substituting from (3.63) and (3.64), this becomes an inhomogeneous second-order ordinary differential equation of Cauchy-Euler type:

$$\begin{aligned} (\lambda + 2\mu)(u_1'' + u_1'/r - u_1/r^2) = & (1/r^3)(\hat{\nu}_2 + \hat{\nu}_3 - \lambda - \mu)b^2/(4\pi^2) \\ & + (1/r^5)(2\hat{\nu}_2 + 4\hat{\nu}_3 - \lambda - 5\mu)4\chi^2 R_0^4. \end{aligned} \quad (3.66)$$

The homogeneous general solution to this equation is of the form $u_{1H} = C_1 r + C_2/r$. The particular solution u_{1P} can be found using Lagrange's method (i.e., variation of parameters). The total general solution is the sum $u_1 = u_{1H} + u_{1P}$:

$$u_1(r) = C_1 r + \frac{C_2}{r} + \frac{b^2(\lambda + \mu - \hat{\nu}_2 - \hat{\nu}_3)}{8\pi^2(\lambda + 2\mu)} \frac{\ln r}{r} + \frac{\chi^2 R_0^4(2\hat{\nu}_2 + 4\hat{\nu}_3 - \lambda - 5\mu)}{2(\lambda + 2\mu)r^3}. \quad (3.67)$$

Consistent with previous arguments, applying vanishing second-order traction end conditions $(\sigma_1)_{rr} = -\tau_{rr}$ at $r = r_0$ and $r = R_0$ gives

$$\begin{aligned} C_1 = & \frac{b^2}{8\pi^2} \left[\frac{\mu(\lambda + \mu - \hat{\nu}_2 - \hat{\nu}_3)}{(\lambda + \mu)(\lambda + 2\mu)} \frac{\ln(R_0/r_0)}{R_0^2 - r_0^2} \right] - \nu s_1' \\ & + \frac{\chi^2 \mu}{2(\lambda + \mu)^2} [(1 - 2\nu)(9\lambda + 9\mu - 2\hat{\nu}_1 - 6\hat{\nu}_2 - 4\hat{\nu}_3) \\ & + 2(\lambda + 5\mu - 2\hat{\nu}_2 - 4\hat{\nu}_3)(R_0^2/r_0^2)], \end{aligned} \quad (3.68)$$

$$C_2 = \frac{b^2}{8\pi^2} \left[\frac{\hat{\nu}_2 - \lambda}{2\mu} + (\lambda + \mu - \hat{\nu}_2 - \hat{\nu}_3) \left(\frac{1}{2\mu} + \frac{r_0^2 \ln R_0 - R_0^2 \ln r_0}{(\lambda + 2\mu)(R_0^2 - r_0^2)} \right) \right] \\ + \chi^2 R_0^2 \left[\frac{(1 - 2\nu)(4\lambda + 14\mu - 4\hat{\nu}_2 - 8\hat{\nu}_3)}{2\mu} + \frac{(\lambda + 5\mu - 2\hat{\nu}_2 - 4\hat{\nu}_3)(R_0^2 + r_0^2)}{2(\lambda + 2\mu)r_0^2} \right]. \quad (3.69)$$

Since σ_1 and τ do not depend on θ and since $(\sigma_1)_{\theta z} = \tau_{\theta z} = 0$, the second-order circumferential equilibrium equation in (3.58) is trivially satisfied. The second-order (i.e., proportional to k^2) axial equilibrium equation is

$$\partial_z [(\sigma_1)_{zz} + \tau_{zz}] = 0 \Rightarrow (\lambda + 2\mu)s_1'' = 0. \quad (3.70)$$

Its general solution is, upon imposing $s_1(0) = 0$ to fix translational invariance,

$$s_1 = C_3 z. \quad (3.71)$$

Therefore, $s_1' = C_3 = \text{constant}$, and Cauchy stress is of the form $\sigma = \sigma(r)$. For an infinite dislocation line ($L \rightarrow \infty$), the second of (3.43) requires $C_3 = 0$. For the first condition in (3.43), corresponding to a dislocation of finite length with $p = 0$, applying the null axial force condition over any cross section normal to the dislocation line:

$$\int_{-\pi}^{\pi} \int_{r_0}^{R_0} [(\sigma_1)_{zz} + \tau_{zz}] r dr d\theta = 0 \quad (3.72)$$

results in an algebraic equation for C_3 that yields

$$C_3 = \frac{b^2}{4\pi^2} \left[\frac{\ln(R_0/r_0)}{R_0^2 - r_0^2} \right] \left[\frac{\lambda + \mu}{\mu(3\lambda + 2\mu)} \right] \\ \times \left[\frac{\lambda(\hat{\nu}_2 + \hat{\nu}_3 - \lambda - \mu)}{\lambda + 2\mu} + \lambda + 4\mu - \hat{\nu}_2 - 2\hat{\nu}_3 - \frac{\lambda\mu(\lambda + \mu - \hat{\nu}_2 - \hat{\nu}_3)}{(\lambda + \mu)(\lambda + 2\mu)} \right]. \quad (3.73)$$

Recall that $(\sigma_0)_{zz} = 0$ when $p = 0$, so that the total axial force from terms proportional to k and k^2 vanishes in this case as well. Since $s_1' = C_3$, solutions for C_1 and C_2 are complete and u_1 (3.67) is fully known, as is second-order Cauchy stress σ_1 in (3.63).

Combining first- and second-order solutions for displacement, (3.38) becomes

$$u(r) = k \left[\chi(1 - 2\nu)r + \frac{\chi R_0^2}{r} \right] \\ + k^2 \left[C_1 r + \frac{C_2}{r} + \frac{b^2(\lambda + \mu - \hat{\nu}_2 - \hat{\nu}_3)}{8\pi^2(\lambda + 2\mu)} \frac{\ln r}{r} + \frac{\chi^2 R_0^4(2\hat{\nu}_2 + 4\hat{\nu}_3 - \lambda - 5\mu)}{2(\lambda + 2\mu)r^3} \right]; \quad (3.74)$$

$$w(\theta) = kb\theta/(2\pi), \quad \theta \in (-\pi, \pi); \quad (3.75)$$

$$s(z) = k^2 C_3 z. \quad (3.76)$$

Recall from (3.35) that $kb = \tilde{b}$ and $kp = \tilde{p}$, and from (3.62) that $\chi \propto p$. All terms in the solution linear in k are proportional to b or χ . All terms in the solution quadratic in k are proportional to b^2 or χ^2 . Therefore, k does not affect the final solution.

Combining first- and second-order solutions for Cauchy stress, (3.36) becomes

$$\sigma(r) = k\sigma_0(r) + k^2[\sigma_1(r) + \tau(r)], \quad (3.77)$$

where σ_0 is given by (3.59) with all terms linear in b or χ , and σ_1 and τ are given by (3.63) and (3.64), respectively, with all terms quadratic in b or χ or bilinear in $b\chi$.

Strain energy per unit reference volume \hat{W} of (3.47) can be written

$$\hat{W} = \frac{1}{2} k^2 \sigma_0 : D_0 + k^3 \sigma_0 : D_1 + \frac{1}{6} k^3 \hat{C}^{ABCDEFGH} D_0_{AB} D_0_{CD} D_0_{EF} + O(k^4), \quad (3.78)$$

where D_0 is the first-order (linear in k) part of strain in (3.45):

$$D_0 = u_0' E_R \otimes E_R + (u_0/r) E_\Theta \otimes E_\Theta + [b/(4\pi r)] (E_\Theta \otimes E_Z + E_Z \otimes E_\Theta), \quad (3.79)$$

and $k^2 \mathbf{D}_1 = \mathbf{D} - k \mathbf{D}_0$ is the second-order part of strain. Considered here is the infinitely extended dislocation line. The first term in (3.78) is computed as

$$\frac{1}{2} \boldsymbol{\sigma}_0 : \mathbf{D}_0 = \mu b^2 / (8\pi^2 r^2) + 2\mu \chi^2 [(1 - 2\nu) + R_0^4 / r^4]. \quad (3.80)$$

Assuming contributions from higher-order products of radial displacement and its derivatives are small compared to those involving shear, second and third terms are

$$\boldsymbol{\sigma}_0 : \mathbf{D}_1 \approx -\mu b^2 \chi (1 + R_0^2 / r^2) / (4\pi^2 r^2), \quad (3.81)$$

$$\frac{1}{6} \hat{C}^{ABCDEF} D_{0AB} D_{0CD} D_{0EF} \approx \frac{b^2 \chi}{4\pi^2 r^2} \left[(1 - 2\nu)(\hat{\nu}_2 + \hat{\nu}_3) + \hat{\nu}_3 \frac{R_0^2}{r^2} \right]. \quad (3.82)$$

Strain energy per unit current volume is \hat{W}/J where J^{-1} is given by (3.42); integrating this over the cross section gives the energy per unit length Ψ , where $\tilde{\chi} = k\chi$:

$$\begin{aligned} \Psi &= \int_{\theta=-\pi}^{\theta=\pi} \int_{r=r_0}^{r=R_0} J^{-1} \hat{W} r dr d\theta \\ &\approx \frac{\tilde{b}^2}{4\pi} \ln \frac{R_0}{r_0} \{ \mu [1 - 2\tilde{\chi}(1 - 2\nu)] + 2\tilde{\chi}(1 - 2\nu)(\hat{\nu}_2 + \hat{\nu}_3 - \lambda - \mu) \} \\ &\quad + 2\pi \tilde{\chi}^2 (R_0^2 - r_0^2) (1 - 2\nu)^2 (\lambda + \mu) [1 - 2\tilde{\chi}(1 - 2\nu)] \\ &\quad + 2\pi \tilde{\chi} (R_0^2 / r_0^2 - 1) \{ b^2 (\hat{\nu}_3 - \mu) / (8\pi^2) + \tilde{\chi} \mu R_0^2 [1 - 2\tilde{\chi}(1 - 2\nu)] \}. \end{aligned} \quad (3.83)$$

The linear elastic energy per unit length is recovered by setting $\tilde{b}^2 \tilde{\chi}, \tilde{\chi}^3 \rightarrow 0$; when core pressure vanishes, this linear solution is the conventional $\Psi = [\mu \tilde{b}^2 / (4\pi)] \ln(R_0 / r_0)$.

3.3 Solution for ideal crystal with Cauchy symmetry

The complete solution depends on 9 parameters: geometric constants (\tilde{b}, r_0, R_0) , elastic constants $(\lambda, \mu, \hat{\nu}_1, \hat{\nu}_2, \hat{\nu}_3)$, and core boundary condition \tilde{p} . The solution is further examined for a reduced set of parameters. Choosing $\tilde{b} = r_0$ [56], the geometry and core pressure become respective functions of dimensionless parameters Λ and p_0 :

$$\Lambda = R_0 / r_0 = R_0 / \tilde{b} > 1, \quad p_0 = \tilde{p} / K. \quad (3.84)$$

Imposing Cauchy symmetry on the elastic constants, which is a physically reasonable assumption for alkali metals and ionic crystals such as the alkali halides [40], produces relations (C.20) and (C.22) of Appendix C (See Supplementary Material, Wiley online library). The number of elastic constants is now two, the linear bulk modulus K and pressure derivative of tangent bulk modulus $K' = B'_0$:

$$\lambda = \mu = \frac{3}{5} K, \quad \hat{\nu}_1 = -\frac{9K}{35} K', \quad \hat{\nu}_2 = -\frac{K}{5} \left(\frac{9}{7} K' - 6 \right), \quad \hat{\nu}_3 = -\frac{K}{5} \left(\frac{9}{7} K' - 9 \right). \quad (3.85)$$

Thus $\nu = \frac{1}{4}$ and all other elastic constants are proportional to K . Typical values for K' in natural crystalline solids are $2 < K' < 7$ [45], with $K' \approx 4$ a common approximation if high pressure data are unavailable. The reduced set of 5 parameters entering the solution is now $(\tilde{b}, \Lambda, p_0, K, K')$. Noting that $\chi = \frac{5}{6} p_0 / (\Lambda^2 - 1)$ and that all coefficients of displacement depend only on dimensionless ratios of elastic constants, normalized displacement \mathbf{u}/\tilde{b} depends only the set of 3 parameters (Λ, p_0, K') . Since stress components and strain energy are linearly proportional to an elastic constant, dimensionless stress and energy $\boldsymbol{\sigma}/K$ and Ψ/K also depend only on this set. It was verified that the dimensionless solution does not depend on \tilde{b} or its units.

Normalized radial displacement $u/r_0 = u/\tilde{b}$ is shown versus Eulerian radial coordinate r in Fig. 1. In this and all later plots of results versus radial coordinate, the abscissa begins at its minimum valid value $r/r_0 = 1$. The effect of core pressure is shown in Fig. 1(a) for a fixed cylinder size of $\Lambda = R_0 / r_0 = 100$: dilatation (i.e., radial expansion) increases with increasing p_0 but decreases rapidly with increasing r . The effect of nonlinear elastic constant K' is shown in Fig. 1(b) for a fixed core pressure $p_0 = 0.1$ and an infinitely long dislocation, i.e., fixed ends ($C_3 = 0$): dilatation increases with increasing K' . The effect of K' is shown in Fig. 1(c) for null core pressure but average free axial conditions (3.72): dilatation increases in magnitude with increasing K' , is positive for $K' > 4$, and is negative for $K' < 4$. Values of C_3 computed from (3.73) are shown in the legend; recall that $C_3 > 0$ corresponds to axial extension, while $C_3 < 0$ corresponds

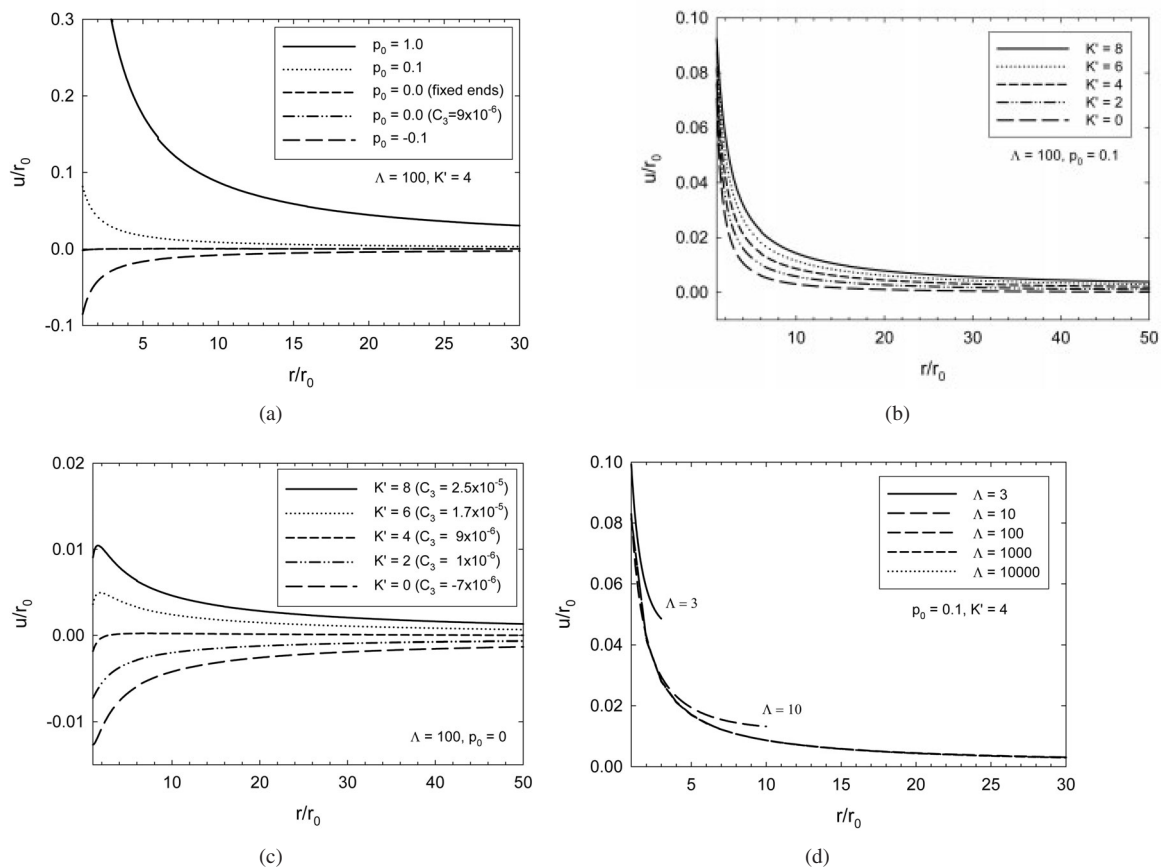


Fig. 1 Total radial displacement for screw dislocation: (a) variable core pressure p_0 (b) variable K' , $p_0 = 0.1$ (c) variable K' , $p_0 = 0$ (d) variable cylinder size $R_0 = \Lambda r_0$.

to axial contraction. For $K' = 4$, $u \approx 0$ for $r > r_0$, suggesting that core pressure rather than elastic nonlinearity may be the primary contributor to dilatation in a typical crystalline solid. Recall in the linear elastic solution $p_0 = 0 \Rightarrow u_0 = 0$. The effect of cylinder size R_0 is shown in Fig. 1(d): for $\Lambda \geq 100$, radial displacements are indistinguishable, while for $\Lambda \leq 10$, increased dilatation is observed since the free surface is closer to the core.

Normalized Cauchy stress field σ/K is shown in Fig. 2 for $\Lambda = 100$ and $K' = 4$. Radial stress is shown in Fig. 2(a); the vertical axis is truncated at $\sigma_{rr} = -0.5K$ since $\sigma_{rr} = -Kp_0$ at $r = r_0$. Maximum magnitudes at $r = r_0$ are on the order of $|p_0|$. Radial and circumferential stress components are of opposite sign and decay rapidly within $r \lesssim 15r_0$. Axial components are negative close to the core and slightly positive farther away from the core, and decrease rapidly within $r \lesssim 5r_0$. All stresses converge towards a single curve for each component for $r \gtrsim 20r_0$ that corresponds to the linear elastic solution with vanishing core pressure. For large r , normal stresses decay to zero and shear stress $\sigma_{\theta z}$ [Fig. 2(d)] is proportional to $1/r$.

Nonlinear and linear solutions for stress and energy per unit length are compared in Fig. 3 and Table 1, respectively. Stress components shown in Fig. 3 correspond to fixed parameters $\Lambda = 100$, $p_0 = 0.1$ (linear and nonlinear) and $K' = 4$ (nonlinear). Radial and circumferential stresses obtained from the nonlinear solution are nearly indistinguishable from corresponding stresses from the linear solution. Axial stress is negative and larger in magnitude for the nonlinear solution compared to the linear solution for $r < 4r_0$. Shear stress is of the same positive sign but smaller in magnitude for the

Table 1 Strain energy $\Psi/(\pi R_0^2 K) \times 10^5$ for screw dislocation, $\Lambda = 100$.

p_0	$K' = 0$	$K' = 2$	$K' = 4$	$K' = 6$	$K' = 8$	linear
1.0	0.929	0.918	0.906	0.896	0.885	0.903
0.1	0.809	0.798	0.787	0.776	0.765	0.783
0.0	0.700	0.700	0.700	0.700	0.700	0.700
-0.1	0.758	0.769	0.780	0.791	0.801	0.783

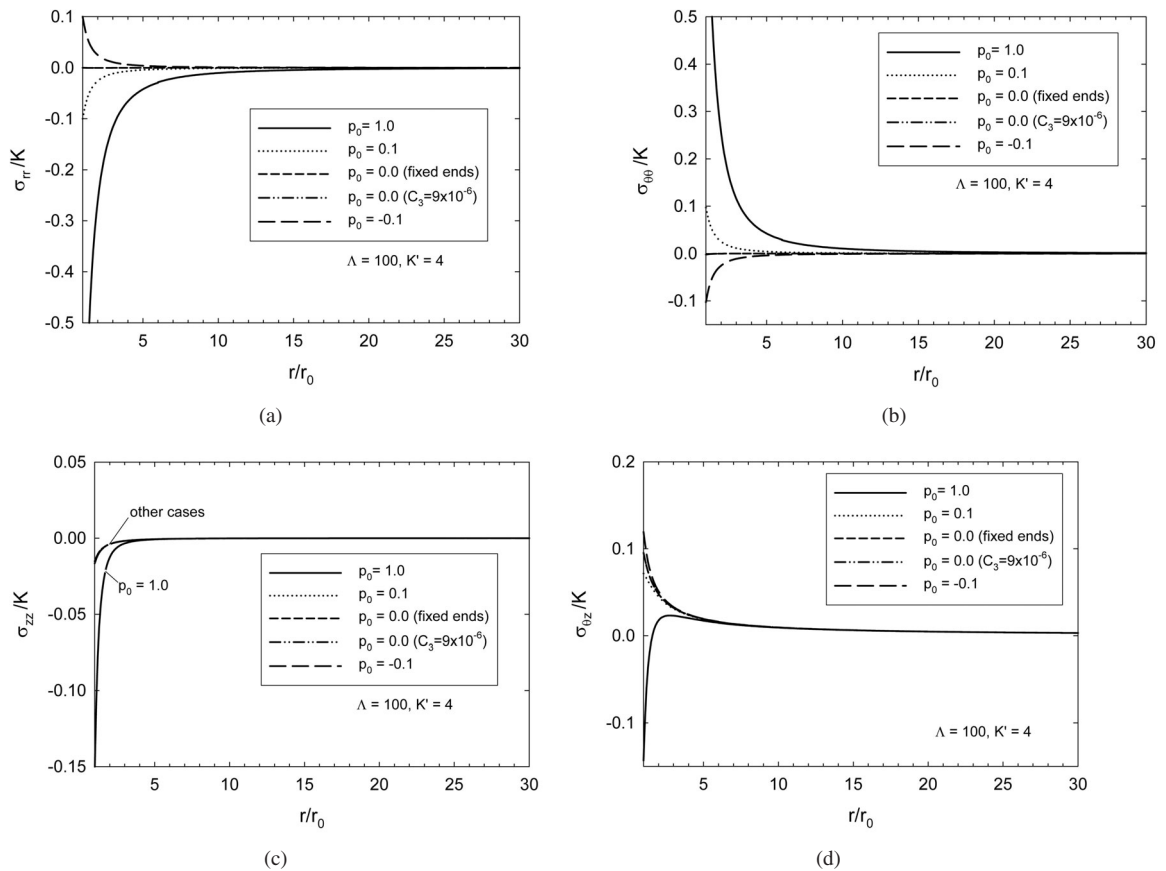


Fig. 2 Cauchy stress field for screw dislocation with $K' = 4$ and $\Lambda = 100$: (a) radial stress (b) circumferential stress (c) axial stress (d) shear stress.

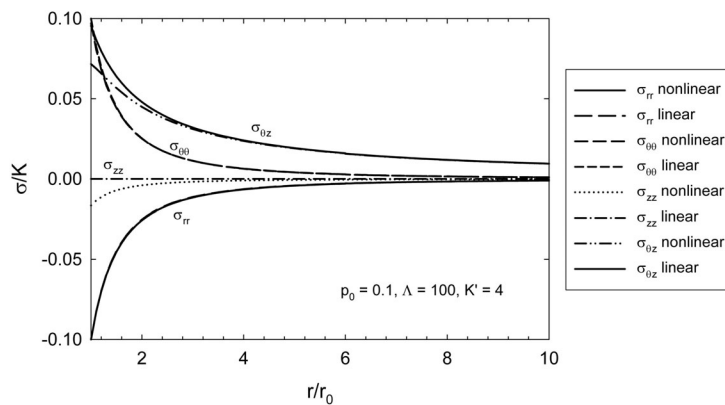


Fig. 3 Comparison of nonlinear and linear elastic solutions for stress field of screw dislocation with $\Lambda = 100$, $p_0 = 0.1$ and $K' = 4$.

nonlinear solution for $r < 4r_0$. The total stress field from the nonlinear solution becomes indistinguishable from the linear solution for $r \gtrsim 10r_0$. Solutions for normalized strain energy in Table 1 are obtained using (3.83), where terms $\propto k^3$ are omitted in the linear solution. For $p_0 = 0$, K' does not affect the solution, and nonlinear and linear predictions coincide. For other values of core pressure, energy predicted using the nonlinear solution may exceed the linear solution depending on the value of K' .

4 Wedge disclination

4.1 Geometric description

Consider a deformed body \mathfrak{B} with boundary $\partial\mathfrak{B}$. In the reference configuration, the image of this body and its boundary are \mathfrak{B}_0 and $\partial\mathfrak{B}_0$. Notation for cylindrical and Cartesian coordinate systems is the same as that used in Sect. 3 and Appendix A (See Supplementary Material, Wiley online library).

An Eulerian description of deformation is invoked, similar to that of Vladimirov et al. [86], though a different strain energy potential and core boundary conditions will be used here. Let the unit tangent line of the disclination be oriented along the z -axis, i.e., $\xi = g_z$. The general ansatz for deformation due to a wedge disclination in an isotropic body is

$$R(r) = r - u(r), \quad \Theta(\theta) = \theta - \hat{\omega}\varphi/(2\pi), \quad Z(z) = z - s(z). \quad (4.1)$$

Radial displacement is $u(r)$, and $\hat{\omega}$ is a constant associated with the Frank vector. When $\hat{\omega} > 0$, the wedge disclination is labeled “positive”, corresponding to removal of a wedge of material and tensile circumferential stress. When $\hat{\omega} < 0$, the disclination is “negative”, corresponding to insertion of a wedge of material and compressive circumferential stress. Angle θ is multi-valued upon complete revolutions around the disclination line, and $\varphi \in (-\pi, \pi)$ is defined in (3.2). Surface \mathfrak{S} , where $\Theta(\theta)$ is discontinuous, corresponds to the half-plane ($y = 0, x < 0$), or $\theta = \pm\pi$. On $\mathfrak{B} \setminus \mathfrak{S}$, the second of (4.1) can be inverted to $\theta = \kappa\Theta$, where $\kappa = 2\pi/(2\pi - \hat{\omega})$.

Displacement $\mathbf{u} = \mathbf{x} - \mathbf{X}$ in (A.38) in physical curvilinear basis $\{\mathbf{e}_a(\theta)\}$ is

$$\mathbf{u} = \{r - (r - u) \cos[\hat{\omega}\varphi/(2\pi)]\}\mathbf{e}_r + \{(r - u) \sin[\hat{\omega}\varphi/(2\pi)]\}\mathbf{e}_\theta + s\mathbf{e}_z. \quad (4.2)$$

Displacement is continuous except for that due to the jump in φ across \mathfrak{S} :

$$[\![\Theta]\!] = \Theta|_{\theta=\pi} - \Theta|_{\theta=-\pi} = -\hat{\omega}, \quad (4.3)$$

$$[\![\mathbf{u}]\!] = \mathbf{u}|_{\theta=\pi} - \mathbf{u}|_{\theta=-\pi} = (u - r)\{[\![\cos[\hat{\omega}\varphi/(2\pi)]]\!]\mathbf{e}_r - [\![\sin[\hat{\omega}\varphi/(2\pi)]]\!]\mathbf{e}_\theta\}. \quad (4.4)$$

For small u and small $\hat{\omega}$, this reduces to the usual approximation $[\![\mathbf{u}]\!] \approx r\hat{\omega}\mathbf{e}_\theta$ [14, 32].

In curvilinear coordinates, the inverse deformation gradient from (4.1) is

$$\begin{aligned} \mathbf{F}^{-1} &= F^{-1R}_{,r} \mathbf{G}_R \otimes \mathbf{g}^r + F^{-1\Theta}_{,\theta} \mathbf{G}_\Theta \otimes \mathbf{g}^\theta + F^{-1Z}_{,z} \mathbf{G}_Z \otimes \mathbf{g}^z \\ &= (dR/dr) \mathbf{G}_R \otimes \mathbf{g}^r + [1 - \hat{\omega}\partial_\theta\varphi/(2\pi)] \mathbf{G}_\Theta \otimes \mathbf{g}^\theta + (dZ/dz) \mathbf{G}_Z \otimes \mathbf{g}^z \\ &= [1 - u'(r)] \mathbf{G}_R \otimes \mathbf{g}^r + [1 - \hat{\omega}\partial_\theta\varphi/(2\pi)] \mathbf{G}_\Theta \otimes \mathbf{g}^\theta + [1 - s'(z)] \mathbf{G}_Z \otimes \mathbf{g}^z. \end{aligned} \quad (4.5)$$

Applying the generalized derivative from (3.5),

$$F^{-1\Theta}_{,\theta} = 1 - [\hat{\omega}/(2\pi)][-r \sin \theta \partial_x \varphi + r \cos \theta \partial_y \varphi] = 1 - \hat{\omega}/(2\pi) + \hat{\omega}rH(-x)\delta(y). \quad (4.6)$$

Define the function $w(\theta)$ and its derivative

$$w = \hat{\omega}\theta/(2\pi), \quad w' = dw/d\theta = \hat{\omega}/(2\pi). \quad (4.7)$$

To fix translational invariance of the origin and ensure volume remains positive,

$$u(0) = 0, \quad s(0) = 0; \quad (1 - u/r)(1 - u')(1 - w')(1 - s') > 0. \quad (4.8)$$

Physically, constraint $|\hat{\omega}| < 2\pi$ also applies.

The multiplicative decomposition of lattice deformation in the first of (2.46) is now applied:

$$\mathbf{F} = \mathbf{F}^E \mathbf{F}^I, \quad \mathbf{F}^{-1} = \mathbf{F}^{I-1} \mathbf{F}^{E-1}. \quad (4.9)$$

The “elastic” part of \mathbf{F}^{-1} is defined as that which, in curvilinear coordinates, is continuous and single-valued over \mathfrak{B} :

$$\mathbf{F}^{E-1} = [1 - u'(r)] \mathbf{G}_R \otimes \mathbf{g}^r + [1 - w'] \mathbf{G}_\Theta \otimes \mathbf{g}^\theta + [1 - s'(z)] \mathbf{G}_Z \otimes \mathbf{g}^z. \quad (4.10)$$

It follows from (4.5), (4.6), and (4.9) that

$$\mathbf{F}^{-1} = \hat{\omega}rH(-x)\delta(y) \mathbf{G}_\Theta \otimes \mathbf{g}^\theta + \mathbf{F}^{E-1}. \quad (4.11)$$

Decomposition (4.9) implies existence of a locally unstressed intermediate configuration $\tilde{\mathfrak{B}}$ for each material element. Selecting coincident cylindrical coordinate systems on $\tilde{\mathfrak{B}}$ and \mathfrak{B}_0 , such that $\mathbf{g}_\alpha(\mathbf{X}) = \delta_\alpha^A \mathbf{G}_A(\mathbf{X})$ [15], and solving for $F^{1-1\Theta}_{\cdot\Theta} = F^{-1\Theta}_{\cdot\Theta} F^{E\Theta}_{\cdot\Theta}$,

$$\mathbf{F}^{1-1} = \{1 + [2\pi r \hat{\omega} / (2\pi - \hat{\omega})] \mathbf{H}(-x) \delta(y)\} \mathbf{G}_\Theta \otimes \mathbf{G}^\Theta. \quad (4.12)$$

From the above description,

$$\mathbf{F}^{-1}(\mathbf{x}) = \mathbf{F}^{E-1} \quad \forall \mathbf{x} \in \mathfrak{B} \setminus \mathfrak{S}, \quad \mathbf{F}^{-1}(\mathbf{x}) = \mathbf{F}^{1-1} \mathbf{F}^{E-1} \quad \text{on } \mathfrak{S}. \quad (4.13)$$

These can be inverted for $\mathbf{F}(\mathbf{x})$. Since $\Theta(\theta)$ is multi-valued across \mathfrak{S} , the referential image of \mathfrak{S} is not a single half-plane as was the case for the screw dislocation in Sect. 3.

The disclination density is now considered. A spatial density tensor $\boldsymbol{\theta}$ and Frank vector $\hat{\omega}$ of the following forms are consistent with geometry of the problem:

$$\boldsymbol{\theta} = \theta^{zz} \mathbf{g}_z \otimes \mathbf{g}_z = \hat{\omega} \delta(r) \mathbf{g}_z \otimes \mathbf{g}_z = \delta(r) \hat{\omega} \otimes \boldsymbol{\xi}; \quad \hat{\omega} = \hat{\omega} \mathbf{g}_z. \quad (4.14)$$

To complete the description of kinematics, variable \mathbf{Q} entering the connection (2.19) is sought that yields (4.14) when used in (2.28) and (2.30). From the second of (2.33), the only nonvanishing covariant components of curvature in are, in spatial Cartesian coordinates,

$$\hat{R}_{xyxy} = \hat{R}_{yxxy} = -\hat{R}_{xyyx} = -\hat{R}_{yxyx} = -\theta^{zz}. \quad (4.15)$$

From (2.28),

$$\hat{R}_{xyxy} = 2(\hat{\nabla}_{[x} Q_{y][xy]} + \hat{T}_{xy}^{\bullet\bullet a} Q_{a[xy]}) - Q_{x[x}^{\bullet\bullet a} Q_{|y|y]a} + Q_{y[y}^{\bullet\bullet a} Q_{|x|x]a}, \quad (4.16)$$

with summation on index a and $(\cdot)_{[xy]} = \frac{1}{2}[(\cdot)_{xy} - (\cdot)_{yx}]$. Existence of a field \mathbf{Q} that simultaneously obeys (4.14)–(4.16) and all of (2.47) is unproven at present. However, the following approximation⁶ is known:

$$\mathbf{Q} = \hat{\omega} \mathbf{H}(-x) \delta(y) (\mathbf{e}_y \otimes \mathbf{e}_y \otimes \mathbf{e}_x - \mathbf{e}_y \otimes \mathbf{e}_x \otimes \mathbf{e}_y), \quad (4.17)$$

$$Q_{yyx} = -Q_{yxy} = \hat{\omega} \mathbf{H}(-x) \delta(y). \quad (4.18)$$

Then (4.16) becomes

$$\hat{R}_{xyxy} = \partial_x Q_{yxy} - Q_{yx}^{\bullet\bullet y} Q_{yxy} \approx \partial_x Q_{yxy} = -\hat{\omega} \delta(-x) \delta(y) = -\hat{\omega} \delta(r) = -\theta^{zz}, \quad (4.19)$$

where terms of $O(\hat{\omega}^2)$ have been omitted in the approximation, yielding a result consistent with (4.14) and (4.15). In the linear approximation, the contribution to the local Burgers vector from the disclination is, with $\mathbf{n} = \mathbf{g}_z$ in (2.48):

$$d\hat{\mathbf{b}} = d^{-1} \boldsymbol{\epsilon} : (\boldsymbol{\theta} \mathbf{n} \otimes \mathbf{x}) da \approx \hat{\omega} \times \mathbf{x} da = r \hat{\omega} \delta(r) dr d\theta \mathbf{g}_\theta. \quad (4.20)$$

Integral $\int d\hat{\mathbf{b}}$ then vanishes identically for domain a with constant normal \mathbf{g}_z parallel to $\boldsymbol{\xi}$ when the disclination passes through $r = 0$. But if the coordinate system is translated such that $\boldsymbol{\xi}$ intersects planar area a at coordinates $(x_0 = r_0 \cos \theta_0, y_0 = r_0 \sin \theta_0)$, then the disclination density becomes $\theta^{zz} = \hat{\omega} \delta(x - x_0) \delta(y - y_0)$ and $\hat{\mathbf{b}} = \int d\hat{\mathbf{b}} = r_0 \hat{\omega} \mathbf{e}_\theta(\theta_0)$.

4.2 Nonlinear elastic analysis and general solution

A nonlinear elastic boundary value problem for the wedge disclination is constructed as follows. Let body \mathfrak{B} consist of a cylinder of outer radius R_0 with the disclination line located along $r = 0$. A cylindrical core region $r < r_0$ is removed from the body and excluded from the solution domain. The length of the cylinder is L , such that the body is contained within the limits $-\frac{L}{2} \leq z \leq \frac{L}{2}$, though the forthcoming analysis also applies for the case $L \rightarrow \infty$. Plane \mathfrak{S} now consists of the two-sided flat region ($\theta = \pm\pi, r_0 < r < R_0$). Body \mathfrak{B} is multiply connected when it contains this plane (i.e., when it is treated as an annular tube), since θ is multi-valued. Body $\mathfrak{B} \setminus \mathfrak{S}$ is simply connected. Its image in the reference configuration, $\mathfrak{B}_0 \setminus \mathfrak{S}_0$, is simply connected when $\hat{\omega} \geq 0$, but contains an overlap of material across \mathfrak{S}_0 when $\hat{\omega} < 0$.

⁶ This approximation is not fully consistent with the second of (2.47) since $\hat{T}_{xy}^{\bullet\bullet y} = -\frac{1}{2} Q_{yx}^{\bullet\bullet y}$ does not vanish, leading to singular dislocation density $\alpha^{yz} = Q_{yx}^{\bullet\bullet y}$ on \mathfrak{S} . Similar artifacts exist in linear representations of discrete disclination lines [32]. The result is inconsequential here since the elastic solution, which does not depend explicitly on the choice of \mathbf{Q} , is sought only over $\mathfrak{B} \setminus \mathfrak{S}$.

The solution procedure parallels that of the screw dislocation of Sect. 3.2. Equilibrium equations are solved on $\mathfrak{B} \setminus \mathfrak{S}$. From (4.13), in this domain the strain energy function in (2.53) becomes

$$W = W(\mathbf{F}) = \hat{W}[\mathbf{D}(\mathbf{F})] = \bar{W}[\mathbf{E}(\mathbf{F})], \quad (4.21)$$

where \hat{W} is used in the solution that follows. Equations (3.28)–(3.31) apply.

Internal boundary conditions are

$$[[\Theta]] = -\hat{\omega} \quad \text{on} \quad \mathfrak{S}; \quad \mathbf{t}|_{r=r_0} = \boldsymbol{\sigma} \mathbf{n} = \tilde{p} \mathbf{e}_r \Rightarrow \sigma^{rr}|_{r=r_0} = -\tilde{p}. \quad (4.22)$$

The first of (4.22) prescribes a coordinate jump across the plane of discontinuity as given in (4.3). The second of (4.22) assigns traction \mathbf{t} at the core surface corresponding to constant radial Cauchy pressure \tilde{p} , with \mathbf{e}_r a unit vector in the radial direction. Traction along the core must be a uniform pressure to maintain consistency with symmetry in ansatz (4.1). External boundary conditions are

$$\mathbf{t}|_{r=R_0} = \mathbf{0}; \quad \left(\int_{r_0}^{R_0} t^z r dr d\theta \right) \Big|_{z=\pm L/2} = 0 \quad \text{or} \quad s(z) \rightarrow 0 \quad \text{as} \quad L \rightarrow \infty. \quad (4.23)$$

The first of (4.23) prescribes traction free conditions on the surface of the cylinder at $r = R_0$. The second of (4.23) prescribes either null average axial force for a cylinder of finite length, or no average axial strain for an infinite cylinder.

An iterative solution procedure in Eulerian coordinates is invoked, similar to that of Vladimirov et al. [86]. The primary difference between the present isotropic nonlinear elastic analysis of the wedge disclination and that in [86] is that here a different strain energy potential \bar{W} is used. A second difference is that possible core pressure is considered, in contrast to [86] that treated the core in a different way. Core pressure was omitted in prior linear solutions [30, 32]. Equations (3.34), (3.36), and (3.37) apply. Internal boundary conditions are of the assumed form

$$\hat{\omega} = k\omega, \quad \tilde{p} = kp, \quad (4.24)$$

which is justified by the vanishing of $\hat{\omega}$ with \tilde{p} . Displacement (3.34) applied to (4.1) and (4.7) results in

$$u(r) = ku_0(r) + k^2 u_1(r), \quad w(\theta) = kw_0(\theta) = k\omega\theta/(2\pi), \quad s(z) = ks_0(z) + k^2 s_1(z), \quad (4.25)$$

where w is necessarily truncated at first order to satisfy the first of (4.22), with

$$\hat{\omega} = k\omega g_z, \quad \hat{\omega} = k\omega. \quad (4.26)$$

With respect to curvilinear cylindrical bases $\{\mathbf{G}_A, \mathbf{g}^a\}$, the inverse deformation gradient matrix on $\mathfrak{B} \setminus \mathfrak{S}$ is

$$[F^{-1A}_{\cdot a}] = \begin{bmatrix} R' & 0 & 0 \\ 0 & \Theta' & 0 \\ 0 & 0 & Z' \end{bmatrix} = \begin{bmatrix} 1 - ku'_0 - k^2 u'_1 & 0 & 0 \\ 0 & 1 - kw'_0 & 0 \\ 0 & 0 & 1 - ks'_0 - k^2 s'_1 \end{bmatrix}. \quad (4.27)$$

In physical components, i.e., orthonormal bases $\{\mathbf{e}_a, \mathbf{E}_A\}$, (A.36) becomes

$$[F^{-1}_{\langle Aa \rangle}] = \begin{bmatrix} 1 - ku'_0 - k^2 u'_1 & 0 & 0 \\ 0 & (1 - ku_0/r - k^2 u_1/r)(1 - kw'_0) & 0 \\ 0 & 0 & 1 - ks'_0 - k^2 s'_1 \end{bmatrix}, \quad (4.28)$$

noting that $\sqrt{G/g} = R/r = 1 - u/r$. Volume ratio is

$$\begin{aligned} J^{-1} &= (1 - ku'_0 - k^2 u'_1)(1 - ku_0/r - k^2 u_1/r)(1 - kw'_0)(1 - ks'_0 - k^2 s'_1) \\ &= 1 - k(u'_0 + u_0/r + w'_0 + s'_0) + O(k^2). \end{aligned} \quad (4.29)$$

In physical cylindrical components, strain tensor \mathbf{D} is, from (3.28) and (4.28),

$$\mathbf{D} = D_{RR} \mathbf{E}_R \otimes \mathbf{E}_R + D_{\Theta\Theta} \mathbf{E}_\Theta \otimes \mathbf{E}_\Theta + D_{ZZ} \mathbf{E}_Z \otimes \mathbf{E}_Z; \quad (4.30)$$

$$\begin{aligned}
D_{RR} &= ku'_0 + k^2(u'_1 - \tfrac{1}{2}u_0'^2), & D_{ZZ} &= ks'_0 + k^2(s'_1 - \tfrac{1}{2}s_0'^2), \\
D_{\Theta\Theta} &= k(w'_0 + u_0/r) + k^2[u_1/r - \tfrac{1}{2}(u_0/r)^2 - \tfrac{1}{2}w_0'^2 - 2w'_0u_0/r],
\end{aligned} \tag{4.31}$$

where terms $O(k^3)$ have been truncated. Strain energy potential per unit reference volume (C.7) is used, truncated at third order, leading to (3.47) which also applies here. Stress $\hat{\mathbf{S}} = \partial\hat{W}/\partial\mathbf{D}$ is, omitting terms of $O(k^3)$,

$$\hat{\mathbf{S}} = \hat{S}_{RR}\mathbf{E}_R \otimes \mathbf{E}_R + \hat{S}_{\Theta\Theta}\mathbf{E}_\Theta \otimes \mathbf{E}_\Theta + \hat{S}_{ZZ}\mathbf{E}_Z \otimes \mathbf{E}_Z; \tag{4.32}$$

$$\begin{aligned}
\hat{S}_{RR} &= k\{(\lambda + 2\mu)u'_0 + \lambda(u_0/r + w'_0 + s'_0)\} \\
&\quad + k^2\{(\lambda + 2\mu)(u'_1 - u_0'^2/2) + \lambda(u_1/r + s'_1 - \tfrac{1}{2}[(u_0/r)^2 + w_0'^2 + s_0'^2] - 2w'_0u_0/r) \\
&\quad + \tfrac{1}{2}(\hat{\nu}_1 + 6\hat{\nu}_2 + 8\hat{\nu}_3)u_0'^2 + \tfrac{1}{2}(\hat{\nu}_1 + 2\hat{\nu}_2)[(w'_0 + u_0/r)^2 + s_0'^2] \\
&\quad + 2u'_0(u_0/r + w'_0 + s'_0)] + \hat{\nu}_1s'_0(u_0/r + w'_0)\},
\end{aligned} \tag{4.33}$$

$$\begin{aligned}
\hat{S}_{\Theta\Theta} &= k\{(\lambda + 2\mu)(w'_0 + u_0/r) + \lambda(u'_0 + s'_0)\} \\
&\quad + k^2\{(\lambda + 2\mu)(u_1/r - \tfrac{1}{2}[(u_0/r)^2 + w_0'^2] - 2w'_0u_0/r) + \lambda(u'_1 - u_0'^2/2 + s'_1 - s_0'^2/2) \\
&\quad + \tfrac{1}{2}(\hat{\nu}_1 + 6\hat{\nu}_2 + 8\hat{\nu}_3)(w'_0 + u_0/r)^2 \\
&\quad + \tfrac{1}{2}(\hat{\nu}_1 + 2\hat{\nu}_2)[u_0'^2 + s_0'^2 + 2(u'_0 + s'_0)(w'_0 + u_0/r)] + \hat{\nu}_1u'_0s'_0\},
\end{aligned} \tag{4.34}$$

$$\begin{aligned}
\hat{S}_{ZZ} &= k\{(\lambda + 2\mu)s'_0 + \lambda(u'_0 + w'_0 + u_0/r)\} \\
&\quad + k^2\{(\lambda + 2\mu)(s'_1 - s_0'^2/2) + \lambda(u'_1 + u_1/r - \tfrac{1}{2}[u_0'^2 + (u_0/r)^2 + w_0'^2] - 2w'_0u_0/r) \\
&\quad + \tfrac{1}{2}(\hat{\nu}_1 + 6\hat{\nu}_2 + 8\hat{\nu}_3)s_0'^2 \\
&\quad + \tfrac{1}{2}(\hat{\nu}_1 + 2\hat{\nu}_2)[u_0'^2 + (w'_0 + u_0/r)^2 + 2(w'_0 + u'_0 + u_0/r)s'_0] + \hat{\nu}_1u'_0(w'_0 + u_0/r)\}.
\end{aligned} \tag{4.35}$$

Using (4.28) and (4.29), Cauchy stress $\boldsymbol{\sigma} = J^{-1}\mathbf{F}^{-T}\hat{\mathbf{S}}\mathbf{F}^{-1}$ is, omitting terms of $O(k^3)$,

$$\boldsymbol{\sigma} = \sigma_{rr}\mathbf{e}_r \otimes \mathbf{e}_r + \sigma_{\theta\theta}\mathbf{e}_\theta \otimes \mathbf{e}_\theta + \sigma_{zz}\mathbf{e}_z \otimes \mathbf{e}_z; \tag{4.36}$$

$$\begin{aligned}
\sigma_{rr} &= k\{(\lambda + 2\mu)u'_0 + \lambda(u_0/r + w'_0 + s'_0)\} \\
&\quad + k^2\{(\lambda + 2\mu)(u'_1 - u_0'^2/2) + \lambda(u_1/r + s'_1 - \tfrac{1}{2}[(u_0/r)^2 + w_0'^2 + s_0'^2] - 2w'_0u_0/r) \\
&\quad + \tfrac{1}{2}(\hat{\nu}_1 + 6\hat{\nu}_2 + 8\hat{\nu}_3)u_0'^2 + \tfrac{1}{2}(\hat{\nu}_1 + 2\hat{\nu}_2)[(w'_0 + u_0/r)^2 + s_0'^2] \\
&\quad + 2u'_0(u_0/r + w'_0 + s'_0)] + \hat{\nu}_1s'_0(u_0/r + w'_0) \\
&\quad - [(\lambda + 2\mu)u'_0 + \lambda(u_0/r + w'_0 + s'_0)](3u'_0 + u_0/r + w'_0 + s'_0)\},
\end{aligned} \tag{4.37}$$

$$\begin{aligned}
\sigma_{\theta\theta} &= k\{(\lambda + 2\mu)(w'_0 + u_0/r) + \lambda(u'_0 + s'_0)\} \\
&\quad + k^2\{(\lambda + 2\mu)(u_1/r - \tfrac{1}{2}[(u_0/r)^2 + w_0'^2] - 2w'_0u_0/r) + \lambda(u'_1 - u_0'^2/2 + s'_1 - s_0'^2/2) \\
&\quad + \tfrac{1}{2}(\hat{\nu}_1 + 6\hat{\nu}_2 + 8\hat{\nu}_3)(w'_0 + u_0/r)^2 \\
&\quad + \tfrac{1}{2}(\hat{\nu}_1 + 2\hat{\nu}_2)[u_0'^2 + s_0'^2 + 2(u'_0 + s'_0)(w'_0 + u_0/r)] + \hat{\nu}_1u'_0s'_0 \\
&\quad - [(\lambda + 2\mu)(w'_0 + u_0/r) + \lambda(u'_0 + s'_0)](u'_0 + 3u_0/r + 3w'_0 + s'_0)\},
\end{aligned} \tag{4.38}$$

$$\begin{aligned}
\sigma_{zz} &= k\{(\lambda + 2\mu)s'_0 + \lambda(u'_0 + w'_0 + u_0/r)\} \\
&\quad + k^2\{(\lambda + 2\mu)(s'_1 - s_0'^2/2) + \lambda(u'_1 + u_1/r - \tfrac{1}{2}[u_0'^2 + (u_0/r)^2 + w_0'^2] - 2w'_0u_0/r) \\
&\quad + \tfrac{1}{2}(\hat{\nu}_1 + 6\hat{\nu}_2 + 8\hat{\nu}_3)s_0'^2 \\
&\quad + \tfrac{1}{2}(\hat{\nu}_1 + 2\hat{\nu}_2)[u_0'^2 + (w'_0 + u_0/r)^2 + 2(w'_0 + u'_0 + u_0/r)s'_0] + \hat{\nu}_1u'_0(w'_0 + u_0/r) \\
&\quad - [(\lambda + 2\mu)s'_0 + \lambda(u'_0 + u_0/r + w'_0)](u'_0 + u_0/r + w'_0 + 3s'_0)\}.
\end{aligned} \tag{4.39}$$

These stress components are consistent with (3.36). Applying (A.39) in spatial physical components, equilibrium equations $\nabla \cdot \boldsymbol{\sigma} = \mathbf{0}$ reduce to

$$\partial_r \sigma_{rr} + (\sigma_{rr} - \sigma_{\theta\theta})/r = 0, \quad \partial_\theta \sigma_{\theta\theta} = 0, \quad \partial_z \sigma_{zz} = 0. \quad (4.40)$$

Since $w'_0 = \text{constant}$, Cauchy stress depends potentially only on r and z , so the second of (4.40) is trivially satisfied.

First consider equilibrium conditions corresponding to stress components linear in k , i.e., the first of (3.37), where

$$\begin{aligned} \boldsymbol{\sigma}_0(r, z) = & [(\lambda + 2\mu)u'_0 + \lambda(u_0/r + w'_0 + s'_0)]\mathbf{e}_r \otimes \mathbf{e}_r \\ & + [(\lambda + 2\mu)(w'_0 + u_0/r) + \lambda(u'_0 + s'_0)]\mathbf{e}_\theta \otimes \mathbf{e}_\theta \\ & + [(\lambda + 2\mu)s'_0 + \lambda(u'_0 + u_0/r + w'_0)]\mathbf{e}_z \otimes \mathbf{e}_z. \end{aligned} \quad (4.41)$$

The first order (i.e., linear in k) axial equilibrium equation produces, with $s_0(0) = 0$ to fix translational invariance,

$$\partial_z(\sigma_0)_{zz} = 0 \Rightarrow s''_0 = 0 \Rightarrow s_0 = c_3 z, \quad (4.42)$$

where c_3 is a constant determined by boundary conditions on ends of the cylinder. Thus $\boldsymbol{\sigma}_0 = \boldsymbol{\sigma}_0(r)$. The first order radial equilibrium equation becomes

$$(\lambda + 2\mu)(u''_0 + u'_0/r - u_0/r^2) = 2\mu w'_0/r. \quad (4.43)$$

This is an inhomogeneous second-order ordinary differential equation of Cauchy-Euler type, with general solution to the homogeneous equation of the form $c_1 r + c_2/r$ and total solution

$$u_0 = c_1 r + c_2/r + [\mu w'_0/(\lambda + 2\mu)]r \ln r. \quad (4.44)$$

Applying boundary conditions $(\sigma_0)_{rr}|_{r=r_0} = -p$ and $(\sigma_0)_{rr}|_{r=R_0} = 0$, the solution is

$$c_1 = \chi(1 - 2\nu) - w'_0/2 - \nu c_3 - \frac{\mu}{\lambda + 2\mu} w'_0 \frac{R_0^2 \ln R_0 - r_0^2 \ln r_0}{R_0^2 - r_0^2}, \quad (4.45)$$

$$c_2 = \chi R_0^2 - \frac{\lambda + \mu}{\lambda + 2\mu} w'_0 \frac{R_0^2 r_0^2}{R_0^2 - r_0^2} \ln \frac{R_0}{r_0}, \quad \chi = [p/(2\mu)][r_0^2/(R_0^2 - r_0^2)]. \quad (4.46)$$

Substituting into (4.44), radial displacement in the linear solution is

$$\begin{aligned} u_0 = & \left[-\frac{\omega}{4\pi} + (1 - 2\nu)\chi - \nu c_3 - \frac{\omega}{4\pi} \frac{1 - 2\nu}{1 - \nu} \frac{R_0^2 \ln R_0 - r_0^2 \ln r_0}{R_0^2 - r_0^2} \right] r \\ & + \left[\chi R_0^2 - \frac{1}{1 - \nu} \frac{\omega}{4\pi} \frac{R_0^2 r_0^2}{R_0^2 - r_0^2} \ln \frac{R_0}{r_0} \right] \frac{1}{r} + \left[\frac{\omega}{4\pi} \frac{1 - 2\nu}{1 - \nu} \right] r \ln r. \end{aligned} \quad (4.47)$$

Constant $c_3 = s'_0$ can now be determined for either of the conditions in (4.23). For vanishing average axial stress,

$$\int_{\theta=-\pi}^{\theta=+\pi} \int_{r=r_0}^{r=R_0} (\sigma_0)_{zz} r dr d\theta = 0 \Rightarrow c_3 = -2\nu\chi/(1 + \nu), \quad (4.48)$$

meaning that positive core pressure leads to axial contraction for $\nu > 0$. For the infinitely long disclination line, $c_3 = 0$, and the linear elastic stress field is

$$\begin{aligned} (\sigma_0)_{rr} = & \frac{\mu}{1 - \nu} \frac{\omega}{2\pi} \ln r - \frac{\mu}{1 - \nu} \frac{\omega}{2\pi} \frac{R_0^2 \ln R_0 - r_0^2 \ln r_0}{R_0^2 - r_0^2} \\ & - \left[2\mu\chi R_0^2 - \frac{\mu}{1 - \nu} \frac{\omega}{2\pi} \frac{R_0^2 r_0^2}{R_0^2 - r_0^2} \ln \frac{R_0}{r_0} \right] \frac{1}{r^2} + 2\mu\chi, \end{aligned} \quad (4.49)$$

$$\begin{aligned} (\sigma_0)_{\theta\theta} = & \frac{\mu}{1 - \nu} \frac{\omega}{2\pi} (\ln r + 1) - \frac{\mu}{1 - \nu} \frac{\omega}{2\pi} \frac{R_0^2 \ln R_0 - r_0^2 \ln r_0}{R_0^2 - r_0^2} \\ & + \left[2\mu\chi R_0^2 - \frac{\mu}{1 - \nu} \frac{\omega}{2\pi} \frac{R_0^2 r_0^2}{R_0^2 - r_0^2} \ln \frac{R_0}{r_0} \right] \frac{1}{r^2} + 2\mu\chi, \end{aligned} \quad (4.50)$$

$$(\sigma_0)_{zz} = \frac{\nu\mu}{1-\nu} \frac{\omega}{2\pi} (2 \ln r + 1) - \frac{2\nu\mu}{1-\nu} \frac{\omega}{2\pi} \frac{R_0^2 \ln R_0 - r_0^2 \ln r_0}{R_0^2 - r_0^2} + 4\nu\mu\chi. \quad (4.51)$$

This solution agrees with [30] when the core is neglected such that $r_0 \rightarrow 0$ and $\chi = 0$, in which case strain energy per unit length is $\mu(k\omega R_0)^2/[16\pi(1-\nu)]$. All components of σ_0 are linear in ω or χ such that k factors out of the final solution $k\sigma_0$.

Henceforth, only the infinitely extended disclination line geometry is addressed, which corresponds to $s_0 = s_1 = 0$ and $z = Z$, and the solution is independent of z . First-order stresses (linear in k) for this case are (4.49)–(4.51). Now consider equilibrium equations for stress components quadratic in k , i.e., the second of (3.37). From (4.37)–(4.39),

$$\begin{aligned} \sigma_1(r) = & [(\lambda + 2\mu)u'_1 + \lambda u_1/r]e_r \otimes e_r + [(\lambda + 2\mu)u_1/r + \lambda u'_1]e_\theta \otimes e_\theta \\ & + [\lambda(u'_1 + u_1/r)]e_z \otimes e_z, \end{aligned} \quad (4.52)$$

$$\begin{aligned} \tau(r) = & \left\{ \frac{1}{2}(\hat{\nu}_1 + 6\hat{\nu}_2 + 8\hat{\nu}_3 - 7\lambda - 14\mu)u_0'^2 + (\hat{\nu}_1 + 2\hat{\nu}_2 - 4\lambda - 2\mu)u_0'u_0/r \right. \\ & + \frac{1}{2}(\hat{\nu}_1 + 2\hat{\nu}_2 - 3\lambda)(u_0/r)^2 + \frac{1}{2}(\hat{\nu}_1 + 2\hat{\nu}_2 - 3\lambda)w_0'^2 \\ & + (\hat{\nu}_1 + 2\hat{\nu}_2 - 4\lambda - 2\mu)u_0'w_0' + (\hat{\nu}_1 + 2\hat{\nu}_2 - 4\lambda)w_0'u_0/r \left. \right\} e_r \otimes e_r \\ & + \left\{ \frac{1}{2}(\hat{\nu}_1 + 2\hat{\nu}_2 - 3\lambda)u_0'^2 + (\hat{\nu}_1 + 2\hat{\nu}_2 - 4\lambda - 2\mu)u_0'u_0/r \right. \\ & + \frac{1}{2}(\hat{\nu}_1 + 6\hat{\nu}_2 + 8\hat{\nu}_3 - 7\lambda - 14\mu)(u_0/r)^2 + \frac{1}{2}(\hat{\nu}_1 + 6\hat{\nu}_2 + 8\hat{\nu}_3 - 7\lambda - 14\mu)w_0'^2 \\ & + (\hat{\nu}_1 + 2\hat{\nu}_2 - 4\lambda - 2\mu)u_0'w_0' + (\hat{\nu}_1 + 6\hat{\nu}_2 + 8\hat{\nu}_3 - 8\lambda - 16\mu)w_0'u_0/r \left. \right\} e_\theta \otimes e_\theta \\ & + \left\{ \frac{1}{2}(\hat{\nu}_1 + 2\hat{\nu}_2 - 3\lambda)u_0'^2 + (\hat{\nu}_1 - 2\lambda)u_0'u_0/r + \frac{1}{2}(\hat{\nu}_1 + 2\hat{\nu}_2 - \lambda)(u_0/r)^2 \right. \\ & + \frac{1}{2}(\hat{\nu}_1 + 2\hat{\nu}_2 - \lambda)w_0'^2 + (\hat{\nu}_1 - 2\lambda)u_0'w_0' + (\hat{\nu}_1 + 2\lambda)w_0'u_0/r \left. \right\} e_z \otimes e_z. \end{aligned} \quad (4.53)$$

The radial component of second-order equilibrium equation in (3.37) is

$$\partial_r(\sigma_1 + \tau)_{rr} + [(\sigma_1 + \tau)_{rr} - (\sigma_1 + \tau)_{\theta\theta}]/r = 0. \quad (4.54)$$

Substituting from (4.52) and (4.53), this becomes an inhomogeneous second-order ordinary differential equation of Cauchy-Euler type:

$$u_1'' + u_1'/r - u_1/r^2 = B_1/r + B_2/r^3 + B_3/r^5 + B_4(\ln r)/r; \quad (4.55)$$

$$\begin{aligned} B_1 = & -\frac{1}{\lambda + 2\mu} [2c_1c_4(2\hat{\nu}_1 + 10\hat{\nu}_2 + 8\hat{\nu}_3 - 11\lambda - 16\mu) \\ & + c_4^2(2\hat{\nu}_1 + 10\hat{\nu}_2 + 12\hat{\nu}_3 - 13\lambda - 23\mu) - w_0'^2(2\hat{\nu}_2 + 4\hat{\nu}_3 - 2\lambda - 7\mu) \\ & - 4c_1w_0'(\hat{\nu}_2 + 2\hat{\nu}_3 - \lambda - 4\mu) + 2c_4w_0'(\hat{\nu}_1 + 2\hat{\nu}_2 - 4\lambda - \mu)], \end{aligned} \quad (4.56)$$

$$B_2 = -\frac{4}{\lambda + 2\mu} c_2[c_4\mu - w_0'(\hat{\nu}_2 + 2\hat{\nu}_3 - \lambda - 3\mu)], \quad (4.57)$$

$$B_3 = -\frac{4}{\lambda + 2\mu} c_2^2(\lambda + 5\mu - 2\hat{\nu}_2 - 4\hat{\nu}_3), \quad (4.58)$$

$$B_4 = -\frac{4}{\lambda + 2\mu} c_4[c_4(\hat{\nu}_1 + 4\hat{\nu}_2 + 4\hat{\nu}_3 - \frac{11}{2}\lambda - 8\mu) - w_0'(\hat{\nu}_2 + 2\hat{\nu}_3 - \lambda - 4\mu)], \quad (4.59)$$

$$c_4 = \frac{\mu}{\mu + 2\lambda} \frac{\omega}{2\pi} = \frac{1-2\nu}{1-\nu} \frac{\omega}{4\pi}, \quad w_0' = \frac{\omega}{2\pi}. \quad (4.60)$$

The homogeneous general solution to this equation is of the form $C_1r + C_2/r$. The particular solution is found using Lagrange's method, which when added to the homogeneous solution gives the total general solution

$$u_1(r) = C_1r + \frac{C_2}{r} + \frac{A_1}{r^3} + A_2r \ln r + A_3r \ln^2 r + A_4 \frac{\ln r}{r}; \quad (4.61)$$

$$A_1 = B_3/8, \quad A_2 = (2B_1 - B_4)/4, \quad A_3 = B_4/4, \quad A_4 = -B_2/2. \quad (4.62)$$

Consistent with boundary conditions and the second of (4.24), applying the vanishing second-order traction end conditions $(\sigma_1)_{rr} = -\tau_{rr}$ at $r = r_0$ and $r = R_0$ gives

$$C_1 = -\frac{D_1}{2(\lambda + \mu)} + \frac{1}{2(\lambda + \mu)(1 - R_0^2/r_0^2)} \{D_3[1/(R_0 r_0)^2 - 1/r_0^4] \\ + D_4[(R_0^2/r_0^2) \ln R_0 - \ln r_0] + D_5[(R_0^2/r_0^2) \ln^2 R_0 - \ln^2 r_0] \\ + D_6[(\ln R_0)/r_0^2 - (\ln r_0)/r_0^2]\}, \quad (4.63)$$

$$C_2 = \frac{D_2}{2\mu} + \frac{1}{2\mu(1/R_0^2 - 1/r_0^2)} \{D_3[1/R_0^4 - 1/r_0^4] + D_4 \ln(R_0/r_0) \\ + D_5[\ln^2 R_0 - \ln^2 r_0] + D_6[(\ln R_0)/R_0^2 - (\ln r_0)/r_0^2]\}; \quad (4.64)$$

$$D_1 = (\lambda + 2\mu)A_2 + (\hat{\nu}_1 + 2\hat{\nu}_2 - 4\lambda)(2c_1 + c_4)w'_0 - 2\mu(c_1 + c_4)w'_0 \\ + \frac{1}{2}(\hat{\nu}_1 + 2\hat{\nu}_2 - 3\lambda)w_0'^2 + (2\hat{\nu}_1 + 6\hat{\nu}_2 + 4\hat{\nu}_3 - 9\lambda - 9\mu)c_1^2 \\ + (2\hat{\nu}_1 + 8\hat{\nu}_2 + 8\hat{\nu}_3 - 11\lambda - 16\mu)c_1 c_4 + \frac{1}{2}(\hat{\nu}_1 + 6\hat{\nu}_2 + 8\hat{\nu}_3 - 7\lambda - 14\mu)c_4^2, \quad (4.65)$$

$$D_2 = (\lambda + 2\mu)A_4 + 2\mu c_2 w'_0 - 2(2\hat{\nu}_2 + 4\hat{\nu}_3 - 2\lambda - 7\mu)c_1 c_2 \\ - (4\hat{\nu}_2 + 8\hat{\nu}_3 - 3\lambda - 12\mu)c_2 c_4, \quad (4.66)$$

$$D_3 = -2(\lambda + 3\mu)A_1 + \frac{1}{2}(4\hat{\nu}_2 + 8\hat{\nu}_3 - 2\lambda - 10\mu)c_2^2, \quad (4.67)$$

$$D_4 = (\lambda + 2\mu)(A_2 + 2A_3) + \lambda A_2 + 2(2\hat{\nu}_1 + 6\hat{\nu}_2 + 4\hat{\nu}_3 - 9\lambda - 9\mu)c_1 c_4 \\ + 2(\hat{\nu}_1 + 2\hat{\nu}_2 - 4\lambda - \mu)c_4 w'_0 + \frac{1}{2}(5\hat{\nu}_1 + 18\hat{\nu}_2 + 16\hat{\nu}_3 - 25\lambda - 32\mu)c_4^2, \quad (4.68)$$

$$D_5 = 2(\lambda + \mu)A_3 + \frac{1}{2}(3\hat{\nu}_1 + 10\hat{\nu}_2 + 8\hat{\nu}_3 - 15\lambda - 18\mu)c_4^2, \quad (4.69)$$

$$D_6 = -2\mu A_4 - 2(2\hat{\nu}_2 + 4\hat{\nu}_3 - 2\lambda - 7\mu)c_2 c_4. \quad (4.70)$$

Second-order contribution to radial displacement u_1 is now fully determined. The total displacement and stress fields are

$$u(r) = k u_0(r) + k^2 u_1(r), \quad \sigma(r) = k \sigma_0(r) + k^2 [\sigma_1(r) + \tau(r)], \quad (4.71)$$

where u_0 is given by (4.47) with $c_3 = 0$, u_1 by (4.61), σ_0 by (4.49)–(4.51), σ_1 by (4.52), and τ by (4.53). Second-order contributions are proportional to ω^2 , χ^2 , or $\omega\chi$; recalling that $\chi \propto p = \tilde{p}/k$ and $\omega = \tilde{\omega}/k$, k does not affect the final solution.

The complete solution depends on 9 parameters: geometric constants $(\hat{\omega}, r_0, R_0)$, elastic constants $(\lambda, \mu, \hat{\nu}_1, \hat{\nu}_2, \hat{\nu}_3)$, and core boundary condition \tilde{p} . General closed form expressions for stresses and displacements in terms of these parameters have not been obtained due to the algebraic complexity of the solution, but numerical values could be found using a computer program for a fixed set of parameters. Energy per unit length $\Psi = 2\pi \int_{r=r_0}^{r=R_0} J^{-1}(r) \hat{W}(r) r dr$ similarly has not been obtained in closed form, but could be integrated numerically. Further examination of the solution using numerical methods is reserved for future work.

5 Point defect

5.1 Geometric description

Consider a deformed body \mathfrak{B} with boundary $\partial\mathfrak{B}$. In the reference configuration, the image of this body and its boundary are \mathfrak{B}_0 and $\partial\mathfrak{B}_0$. Spherical coordinates covering \mathfrak{B} and \mathfrak{B}_0 are (r, θ, ϕ) and (R, Θ, Φ) and are described fully in Appendix B, including basis vectors; Cartesian coordinates are (x, y, z) and (X, Y, Z) .

An Eulerian description of deformation is invoked, in contrast to previous works that used Lagrangian descriptions [57, 62, 72], and a different strain energy potential (\hat{W} rather than \bar{W}) is also used here. The point defect is treated as a singular center of dilatation or contraction at point $\mathfrak{p} \in \mathfrak{B}$ located at the origin of the spatial coordinate system. This defect could physically correspond to a vacancy, interstitial, or substitutional atom, or an inclusion of small size. The general ansatz for deformation due to a point defect in an isotropic body is of the spherically symmetric form

$$R(r) = r - u(r), \quad \Theta(\theta) = \theta, \quad \Phi(\phi) = \phi. \quad (5.1)$$

Radial displacement is $u(r)$, positive for dilatation and negative for contraction. Rigid body translation is excluded, restricting $u(0) = 0$ such that \mathbf{p}_0 , the referential image of \mathbf{p} , also occupies the origin of the coordinate system on \mathfrak{B}_0 .

In curvilinear coordinates, the inverse deformation gradient from (5.1) is

$$\begin{aligned}\mathbf{F}^{-1} &= F^{-1R} \mathbf{G}_R \otimes \mathbf{g}^r + F^{-1\Theta} \mathbf{G}_\Theta \otimes \mathbf{g}^\theta + F^{-1\Phi} \mathbf{G}_\Phi \otimes \mathbf{g}^\phi \\ &= [1 - u'(r)] \mathbf{G}_R \otimes \mathbf{g}^r + \mathbf{G}_\Theta \otimes \mathbf{g}^\theta + \mathbf{G}_\Phi \otimes \mathbf{g}^\phi.\end{aligned}\quad (5.2)$$

Volume ratio is

$$J^{-1} = (R^2/r^2) \det \mathbf{F}^{-1} = (1 - u')(1 - u/r)^2 > 0, \quad (5.3)$$

noting that $\sqrt{G/g} = R^2/r^2 = (1 - u/r)^2$. Applying the first of (2.49) in curvilinear coordinates,

$$\mathbf{F}^{-1} = \mathbf{F}^{I-1} \mathbf{F}^{E-1} = F^{I-1A} F^{E-1\alpha} \mathbf{G}_A \otimes \mathbf{g}^a. \quad (5.4)$$

The second of (2.50) applied to the singular point defect is, with g_α^A the shifter,

$$\mathbf{F}^{I-1} = J^{I-1/3} \mathbf{g}_\alpha \otimes \mathbf{g}^\alpha = J^{I-1/3} g_\alpha^A \mathbf{G}_A \otimes \mathbf{g}^\alpha, \quad F^{I-1A} = J^{I-1/3} g_\alpha^A; \quad (5.5)$$

$$J^{I-1} = 1 - \delta v \delta(x) \delta(y) \delta(z) = 1 - \delta v \delta(r). \quad (5.6)$$

Inelastic volume change induced by the defect is measured by scalar constant δv that can be positive or negative. The spherical Dirac delta function is $\delta(r) = \delta(x) \delta(y) \delta(z)$, differing from that used for cylindrical coordinates in Sect. 3 and Sect. 4. Therefore,

$$\mathbf{F}(\mathbf{X}) = \mathbf{F}^E(\mathbf{X}) \quad \forall \mathbf{X} \in \mathfrak{B}_0 \setminus \mathbf{p}_0, \quad \mathbf{F}^{-1}(\mathbf{x}) = \mathbf{F}^{E-1}(\mathbf{x}) \quad \forall \mathbf{x} \in \mathfrak{B} \setminus \mathbf{p}. \quad (5.7)$$

Vector $\boldsymbol{\vartheta}$ entering Burgers vector integral (2.52) is of the spherically symmetric form $\boldsymbol{\vartheta} = \iota(r) \delta(r) \mathbf{g}_r$. For an area element of a spherical shell with unit normal \mathbf{g}_r , the differential form of (2.52) is $d\mathbf{b}(r) = \iota(r) \delta(r) r \mathbf{g}_r da = \iota(r) \delta(r) r^3 \sin \theta d\theta d\phi \mathbf{g}_r$. Integral $\int d\mathbf{b}$ then vanishes identically for a point defect at $r = 0$, but does not always vanish for a different coordinate system, similarly to the case for the disclination in Sect. 4.1.

5.2 Nonlinear elastic analysis and general solution

A nonlinear elastic boundary value problem for the point defect is constructed as follows. Let body \mathfrak{B} consist of an elastic sphere of outer radius R_0 with the ball $0 \leq r < r_0$ removed. Body \mathfrak{B} is simply connected, as is its image in the reference configuration, \mathfrak{B}_0 . Region $r < r_0$ is called the core of the point defect, and is elastically rigid, i.e., $\mathbf{F}^E = \mathbf{1}$ for $r < r_0$. Deformation of the core region is inelastic or residual:

$$\mathbf{F}^{-1}|_{r < r_0} = \mathbf{F}^{I-1} = J^{I-1/3} \mathbf{g}_a \otimes \mathbf{g}^a, \quad J^I = \det \mathbf{F}^I, \quad (5.8)$$

where the determinant applies in a coincident spatial basis $\{\mathbf{g}_a, \mathbf{g}^a\}$ [15]. Spatial volume of the defect core is $v_0 = \frac{4}{3} \pi r_0^3$; referential volume of the core is, from (5.6),

$$V_0 = \int_{v_0} J^{I-1} dv = \int_{v_0} [1 - \delta v \delta(r)] dv = v_0 - \delta v. \quad (5.9)$$

Displacement boundary conditions are imposed on the elastic body at its inner surface $r = r_0$ such that the volume of a spherical shell of radius r_0 and constant thickness $\hat{\eta}$ is equal to the volume change induced by the core:

$$\delta v = 4\pi r_0^2 \hat{\eta}, \quad \hat{\eta} = u(r_0). \quad (5.10)$$

Condition $\hat{\eta} > 0$ corresponds to a referential core of radius smaller than r_0 , leading to radial expansion of the surrounding elastic medium in the current configuration. Conversely, $\hat{\eta} < 0$ corresponds to a referential core of radius larger than r_0 , leading to radial contraction of the surrounding elastic medium in the current configuration. Requiring $V_0 > 0$ leads to constraint $\hat{\eta} < r_0/3$.

The solution procedure parallels that of Sect. 4.2, with spherical rather than cylindrical symmetry. Equilibrium equations are solved on \mathfrak{B} , which excludes region $r < r_0$ and therefore excludes singular point \mathbf{p} . From (5.7), in this domain the strain energy function in (2.53) becomes

$$W = W(\mathbf{F}) = \hat{W}[\mathbf{D}(\mathbf{F})] = \bar{W}[\mathbf{E}(\mathbf{F})], \quad (5.11)$$

where \hat{W} is used in the solution that follows. Equations (3.28)–(3.31) apply. Internal and external boundary conditions are

$$u|_{r=r_0} = \hat{\eta}, \quad \mathbf{t}|_{r=R_0} = (\sigma^{rr}|_{r=R_0})\mathbf{g}_r = \mathbf{0}. \quad (5.12)$$

The first of (5.12) prescribes radial displacement at the core consistent with inelastic volume change of the core. The second of (5.12) enforces vanishing traction on the external part of $\partial\mathfrak{B}$.

An iterative solution procedure in Eulerian coordinates is invoked. Equations (3.34), (3.36), and (3.37) apply. Internal boundary conditions are of the form

$$\hat{\eta} = k\eta. \quad (5.13)$$

Displacement (3.34) applied to (5.1) results in

$$u(r) = ku_0(r) + k^2u_1(r). \quad (5.14)$$

In physical components, i.e., orthonormal bases $\{\mathbf{e}_a, \mathbf{E}_A\}$, (5.2) and (B.36) become

$$[F^{-1}_{\langle Aa \rangle}] = \begin{bmatrix} R' & 0 & 0 \\ 0 & R/r & 0 \\ 0 & 0 & R/r \end{bmatrix} = \begin{bmatrix} 1 - u' & 0 & 0 \\ 0 & 1 - u/r & 0 \\ 0 & 0 & 1 - u/r \end{bmatrix}. \quad (5.15)$$

Substituting from (5.14),

$$[F^{-1}_{\langle Aa \rangle}] = \begin{bmatrix} 1 - ku'_0 - k^2u'_1 & 0 & 0 \\ 0 & 1 - ku_0/r - k^2u_1/r & 0 \\ 0 & 0 & 1 - ku_0/r - k^2u_1/r \end{bmatrix}, \quad (5.16)$$

and (5.3) becomes

$$J^{-1} = \det[F^{-1}_{\langle Aa \rangle}] = (1 - ku'_0 - k^2u'_1)(1 - ku_0/r - k^2u_1/r)^2 \approx 1 - k(u'_0 + 2u_0/r). \quad (5.17)$$

In physical spherical components, strain tensor \mathbf{D} is, from (3.28) and (5.16),

$$\mathbf{D} = D_{RR}\mathbf{E}_R \otimes \mathbf{E}_R + D_{\Theta\Theta}\mathbf{E}_\Theta \otimes \mathbf{E}_\Theta + D_{\Phi\Phi}\mathbf{E}_\Phi \otimes \mathbf{E}_\Phi; \quad (5.18)$$

$$D_{RR} = ku'_0 + k^2(u'_1 - \frac{1}{2}u_0'^2), \quad D_{\Theta\Theta} = D_{\Phi\Phi} = ku_0/r + k^2[u_1/r - \frac{1}{2}(u_0/r)^2], \quad (5.19)$$

where terms $O(k^3)$ have been truncated. Strain energy potential per unit reference volume (C.7) is used, truncated at third order, leading to (3.47) which also applies here. Stress $\hat{\mathbf{S}} = \partial\hat{W}/\partial\mathbf{D}$ is, omitting terms of $O(k^3)$,

$$\hat{\mathbf{S}} = \hat{S}_{RR}\mathbf{E}_R \otimes \mathbf{E}_R + \hat{S}_{\Theta\Theta}\mathbf{E}_\Theta \otimes \mathbf{E}_\Theta + \hat{S}_{\Phi\Phi}\mathbf{E}_\Phi \otimes \mathbf{E}_\Phi; \quad (5.20)$$

$$\begin{aligned} \hat{S}_{RR} &= k\{(\lambda + 2\mu)u'_0 + 2\lambda u_0/r\} \\ &\quad + k^2\{(\lambda + 2\mu)(u'_1 - u_0'^2/2) + 2\lambda[u_1/r - \frac{1}{2}(u_0/r)^2]\} \\ &\quad + \frac{1}{2}(\hat{\nu}_1 + 6\hat{\nu}_2 + 8\hat{\nu}_3)u_0'^2 + 2(\hat{\nu}_1 + \hat{\nu}_2)(u_0/r)^2 + 2(\hat{\nu}_1 + 2\hat{\nu}_2)u'_0u_0/r\}, \end{aligned} \quad (5.21)$$

$$\begin{aligned} \hat{S}_{\Theta\Theta} = \hat{S}_{\Phi\Phi} &= k\{(2\lambda + 2\mu)u_0/r + \lambda u'_0\} \\ &\quad + k^2\{(2\lambda + 2\mu)[u_1/r - \frac{1}{2}(u_0/r)^2] + \lambda(u'_1 - u_0'^2/2) \\ &\quad + \frac{1}{2}(\hat{\nu}_1 + 2\hat{\nu}_2)u_0'^2 + 2(\hat{\nu}_1 + 3\hat{\nu}_2 + 2\hat{\nu}_3)(u_0/r)^2 + 2(\hat{\nu}_1 + \hat{\nu}_2)u'_0u_0/r\}. \end{aligned} \quad (5.22)$$

Using (5.16) and (5.17), Cauchy stress $\boldsymbol{\sigma} = J^{-1}\mathbf{F}^{-T}\hat{\mathbf{S}}\mathbf{F}^{-1}$ is, omitting terms of $O(k^3)$,

$$\boldsymbol{\sigma} = \sigma_{rr}\mathbf{e}_r \otimes \mathbf{e}_r + \sigma_{\theta\theta}\mathbf{e}_\theta \otimes \mathbf{e}_\theta + \sigma_{\phi\phi}\mathbf{e}_\phi \otimes \mathbf{e}_\phi; \quad (5.23)$$

$$\begin{aligned} \sigma_{rr} &= k\{(\lambda + 2\mu)u'_0 + 2\lambda u_0/r\} \\ &\quad + k^2\{(\lambda + 2\mu)(u'_1 - u_0'^2/2) + 2\lambda[u_1/r - \frac{1}{2}(u_0/r)^2]\} \\ &\quad + \frac{1}{2}(\hat{\nu}_1 + 6\hat{\nu}_2 + 8\hat{\nu}_3)u_0'^2 + 2(\hat{\nu}_1 + \hat{\nu}_2)(u_0/r)^2 + 2(\hat{\nu}_1 + 2\hat{\nu}_2)u'_0u_0/r \\ &\quad - [(\lambda + 2\mu)u'_0 + 2\lambda u_0/r](3u'_0 + 2u_0/r)\}, \end{aligned} \quad (5.24)$$

$$\begin{aligned}
\sigma_{\theta\theta} = \sigma_{\phi\phi} = & k\{(2\lambda + 2\mu)u_0/r + \lambda u'_0\} \\
& + k^2\{(2\lambda + 2\mu)[u_1/r - \frac{1}{2}(u_0/r)^2] + \lambda(u'_1 - u_0'^2/2) \\
& + \frac{1}{2}(\hat{\nu}_1 + 2\hat{\nu}_2)u_0'^2 + 2(\hat{\nu}_1 + 3\hat{\nu}_2 + 2\hat{\nu}_3)(u_0/r)^2 + 2(\hat{\nu}_1 + \hat{\nu}_2)u'_0 u_0/r \\
& - [(2\lambda + 2\mu)u_0/r + \lambda u'_0](u'_0 + 4u_0/r)\}.
\end{aligned} \tag{5.25}$$

These stress components are consistent with (3.36). Applying (B.38) in spatial physical components, equilibrium equations $\nabla \cdot \boldsymbol{\sigma} = \mathbf{0}$ reduce to, in the absence of shear stress,

$$\partial_r \sigma_{rr} + (2\sigma_{rr} - \sigma_{\theta\theta} - \sigma_{\phi\phi})/r = 0, \quad \partial_\theta \sigma_{\theta\theta} + (\sigma_{\theta\theta} - \sigma_{\phi\phi}) \cot \theta = 0, \quad \partial_\phi \sigma_{\phi\phi} = 0. \tag{5.26}$$

Noting that $\boldsymbol{\sigma} = \boldsymbol{\sigma}(r)$ and $\sigma_{\theta\theta} = \sigma_{\phi\phi}$, the second and third equilibrium equations are trivially satisfied, and radial equilibrium becomes

$$d\sigma_{rr}/dr + 2(\sigma_{rr} - \sigma_{\theta\theta})/r = 0. \tag{5.27}$$

First consider equilibrium conditions corresponding to stress components linear in k , i.e., the first of (3.37), where

$$\boldsymbol{\sigma}_0(r) = [(\lambda + 2\mu)u'_0 + 2\lambda u_0/r]\mathbf{e}_r \otimes \mathbf{e}_r + [(2\lambda + 2\mu)u_0/r + \lambda u'_0](\mathbf{e}_\theta \otimes \mathbf{e}_\theta + \mathbf{e}_\phi \otimes \mathbf{e}_\phi). \tag{5.28}$$

First order radial equilibrium equation (5.27) becomes

$$(\lambda + 2\mu)(u_0'' + 2u'_0/r - 2u_0/r^2) = 0. \tag{5.29}$$

This is a homogeneous second-order ordinary differential equation of Cauchy-Euler type with general solution

$$u_0 = c_1 r + c_2/r^2. \tag{5.30}$$

Applying boundary conditions $u_0(r_0) = \eta$ and $(\sigma_0)_{rr}|_{r=R_0} = 0$ consistently with (5.12) and (5.13), the solution is

$$c_1 = \frac{4\mu r_0^2 \eta}{[(3\lambda + 2\mu) + 4\mu(r_0/R_0)^3]R_0^3}, \quad c_2 = \frac{(3\lambda + 2\mu)r_0^2 \eta}{3\lambda + 2\mu + 4\mu(r_0/R_0)^3}. \tag{5.31}$$

First order stresses become

$$(\sigma_0)_{rr} = (3\lambda + 2\mu)c_1 - 4\mu c_2/r^3, \quad (\sigma_0)_{\theta\theta} = (\sigma_0)_{\phi\phi} = (3\lambda + 2\mu)c_1 + 2\mu c_2/r^3. \tag{5.32}$$

First-order pressure is $-\frac{1}{3}\text{tr}\boldsymbol{\sigma}_0 = -3Kc_1$, with $K = \lambda + \frac{2}{3}\mu$ the bulk modulus. Displacement u_0 and stresses (5.32) are linear in $\eta = \hat{\eta}/k$, so k does not affect the solution, which agrees with previous derivations [14, 81]. Strain energy density is

$$\hat{W} = \frac{1}{2}k^2 \boldsymbol{\sigma}_0 : \mathbf{D}_0 + \mathcal{O}(k^3) = \frac{3}{2}k^2[(3\lambda + 2\mu)c_1^2 + 4\mu c_2^2/r^6] + \mathcal{O}(k^3). \tag{5.33}$$

Integrating over \mathfrak{B} and dividing by total volume of the elastic sphere minus core gives the average strain energy density in the linear approximation

$$\frac{3}{4\pi(R_0^3 - r_0^3)} \int_{\mathfrak{B}} J^{-1} \hat{W} dv = \frac{3}{2}k^2[(3\lambda + 2\mu)c_1^2 + 4\mu c_2^2/(R_0 r_0)^3] + \mathcal{O}(k^3). \tag{5.34}$$

Now consider equilibrium equations for stress components quadratic in k , i.e., the second of (3.37). From (5.24) and (5.25),

$$\boldsymbol{\sigma}_1(r) = [(\lambda + 2\mu)u'_1 + 2\lambda u_1/r]\mathbf{e}_r \otimes \mathbf{e}_r + [(2\lambda + 2\mu)u_1/r + \lambda u'_1](\mathbf{e}_\theta \otimes \mathbf{e}_\theta + \mathbf{e}_\phi \otimes \mathbf{e}_\phi), \tag{5.35}$$

$$\begin{aligned}
\boldsymbol{\tau}(r) = & \left\{ \frac{1}{2}(\hat{\nu}_1 + 6\hat{\nu}_2 + 8\hat{\nu}_3 - 7\lambda - 14\mu)u_0'^2 + 2(\hat{\nu}_1 + 2\hat{\nu}_2 - 4\lambda - 2\mu)u'_0 u_0/r \right. \\
& + (2\hat{\nu}_1 + 2\hat{\nu}_2 - 5\lambda)(u_0/r)^2 \left. \right\} \mathbf{e}_r \otimes \mathbf{e}_r \\
& + \left\{ \frac{1}{2}(\hat{\nu}_1 + 2\hat{\nu}_2 - 3\lambda)u_0'^2 + 2(\hat{\nu}_1 + \hat{\nu}_2 - 3\lambda - \mu)u'_0 u_0/r \right. \\
& + (2\hat{\nu}_1 + 6\hat{\nu}_2 + 4\hat{\nu}_3 - 9\lambda - 9\mu)(u_0/r)^2 \left. \right\} (\mathbf{e}_\theta \otimes \mathbf{e}_\theta + \mathbf{e}_\phi \otimes \mathbf{e}_\phi).
\end{aligned} \tag{5.36}$$

Second-order equilibrium equation (5.27) is

$$d(\sigma_1 + \tau)_{rr}/dr + 2[(\sigma_1 + \tau)_{rr} - (\sigma_1 + \tau)_{\theta\theta}]/r = 0. \quad (5.37)$$

Substituting from (5.35) and (5.36), this becomes an inhomogeneous second-order ordinary differential equation of Cauchy-Euler type:

$$u_1'' + 2\frac{u_1'}{r} - 2\frac{u_1}{r^2} = \frac{18(2\hat{\nu}_2 + 4\hat{\nu}_3 - \lambda - 5\mu)c_2^2}{(\lambda + 2\mu)r^7}. \quad (5.38)$$

The general solution to the homogeneous equation is of the form $C_1 r + C_2/r^2$; adding this to the particular solution gives the total solution

$$u_1 = C_1 r + C_2/r^2 + A_1/r^5, \quad A_1 = [(2\hat{\nu}_2 + 4\hat{\nu}_3 - \lambda - 5\mu)c_2^2]/(\lambda + 2\mu). \quad (5.39)$$

Consistent with boundary conditions (5.12) and (5.13), applying second-order end conditions $u_1(r_0) = 0$ and $(\sigma_1)_{rr} = -\tau_{rr}$ at $r = R_0$ gives

$$C_1 = -\frac{A_1}{r_0^6} + \frac{1}{3K + 4\mu(r_0/R_0)^3} \left[\frac{3KA_1}{r_0^6} + B_1 + \frac{B_2}{R_0^3} + \frac{B_3}{R_0^6} \right], \quad (5.40)$$

$$C_2 = -\frac{1}{3K + 4\mu(r_0/R_0)^3} \left[\frac{3KA_1}{r_0^3} + B_1 r_0^3 + \frac{B_2 r_0^3}{R_0^3} + \frac{B_3 r_0^3}{R_0^6} \right]; \quad (5.41)$$

$$B_1 = -\frac{1}{2}c_1^2(9\hat{\nu}_1 + 18\hat{\nu}_2 + 8\hat{\nu}_3 - 33\lambda - 22\mu), \quad (5.42)$$

$$B_2 = 4c_1 c_2(3\hat{\nu}_2 + 4\hat{\nu}_3 - 3\lambda - 8\mu), \quad (5.43)$$

$$B_3 = -c_2^2[6\hat{\nu}_2 + 16\hat{\nu}_3 - 3\lambda(1 + A_1/c_2^2) - 10\mu(2 + A_1/c_2^2)]. \quad (5.44)$$

Second-order contribution to radial displacement u_1 is now fully determined. The total displacement and stress fields are

$$u(r) = ku_0(r) + k^2 u_1(r), \quad \sigma(r) = k\sigma_0(r) + k^2[\sigma_1(r) + \tau(r)], \quad (5.45)$$

where u_0 is given by (5.30), u_1 by (5.39), σ_0 by (5.32), σ_1 by (5.35), and τ by (5.36). Second-order contributions are proportional to η^2 ; recalling that $\eta = \hat{\eta}/k$, k does not affect the final solution.

5.3 Solution for ideal crystal with Cauchy symmetry

The complete solution depends on 8 parameters: geometric constants (r_0, R_0), elastic constants ($\lambda, \mu, \hat{\nu}_1, \hat{\nu}_2, \hat{\nu}_3$), and core boundary condition $\delta v = 4\pi r_0^2 \hat{\eta}$. The solution is further examined for a reduced set of parameters. The geometry and displaced core volume can be expressed in terms of dimensionless parameters Λ and η_0 :

$$\Lambda = R_0/r_0 > 1, \quad \eta_0 = \hat{\eta}/r_0 = \delta v/(4\pi r_0^3) < 1/3. \quad (5.46)$$

Imposing Cauchy symmetry on the elastic constants as in Sect. 3.3, (3.85) applies, which reduces independent elastic constants to K and K' . The reduced set of 5 parameters entering the solution is now $(\Lambda, r_0, \eta_0, K, K')$. Noting that all coefficients of displacement depend only on dimensionless ratios of elastic constants, normalized radial displacement u/r_0 versus r/r_0 depends only the set of 3 parameters (Λ, η_0, K') . Since stress components are linearly proportional to an elastic constant, dimensionless stress σ/K versus r/r_0 also depends only on this set, as does normalized volume change

$$\frac{\Delta V}{\delta v} = \frac{(4/3)\pi R_0^3 - (4/3)\pi[R_0 - u(R_0)]^3}{4\pi r_0^2 \hat{\eta}} = \frac{\Lambda^3 - [\Lambda - u(R_0)/r_0]^3}{3\eta_0}. \quad (5.47)$$

Normalized radial displacement u/r_0 is shown versus Eulerian radial coordinate r in Fig. 4. The effect of core displacement is shown in Fig. 4(a) for an elastic sphere of size $\Lambda = R_0/r_0 = 100$ and $K' = 4$: dilatation (i.e., radial expansion) increases with increasing η_0 but decreases rapidly with increasing r . Recall that $\eta_0 > 0$ corresponds physically to a large substitutional atom or interstitial, while $\eta_0 < 0$ corresponds to a small substitutional atom or vacancy. The effect of non-linear elastic constant K' is shown in Fig. 4(b) for $\eta_0 = 0.3$ and $\eta_0 = -0.3$: dilatation increases with increasing K' for $\eta_0 > 0$ and radial contraction decreases with increasing K' for $\eta_0 < 0$. The effect of sphere size R_0 is shown in Fig. 4(c)

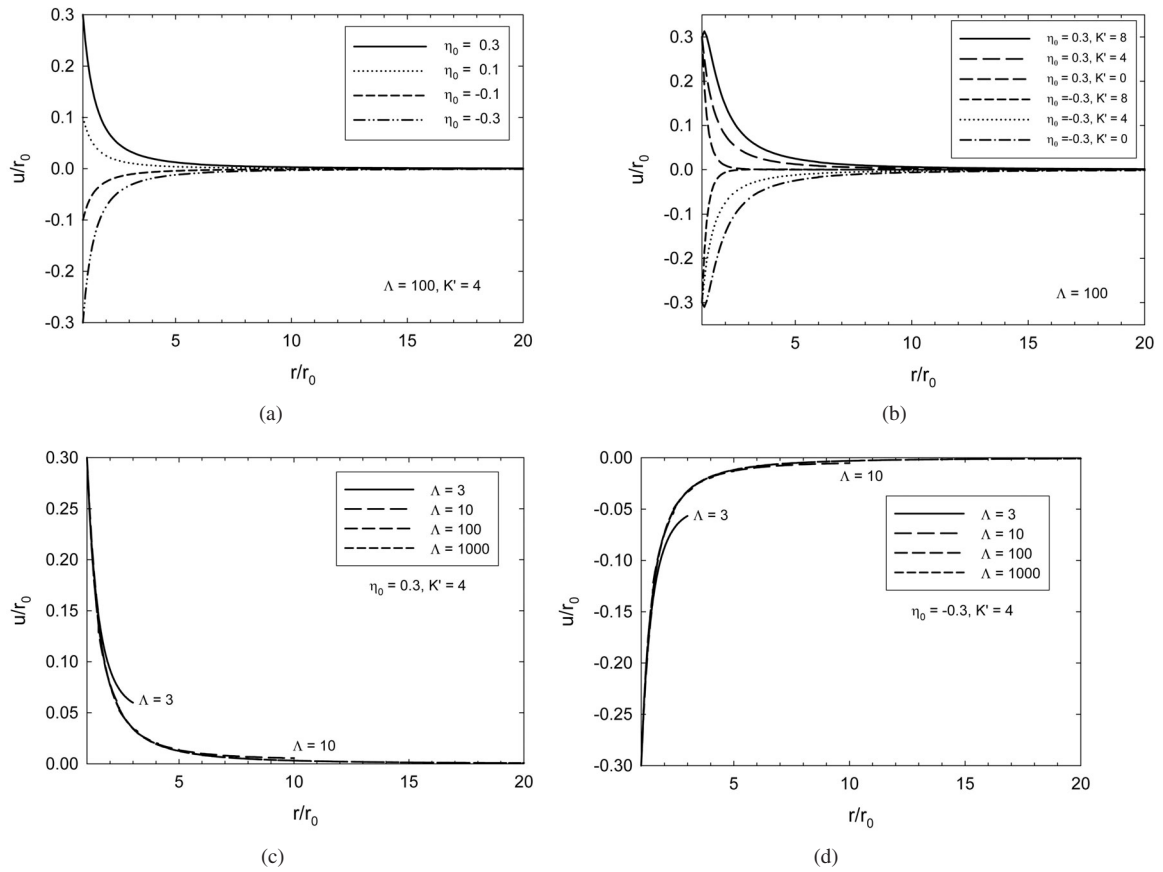


Fig. 4 Total radial displacement for point defect: (a) variable core displacement η_0 (b) variable K' , $\eta_0 = 0.3, -0.3$ (c) variable sphere size $R_0 = \Lambda r_0$ with $\eta_0 = 0.3$ (d) variable sphere size $R_0 = \Lambda r_0$ with $\eta_0 = -0.3$.

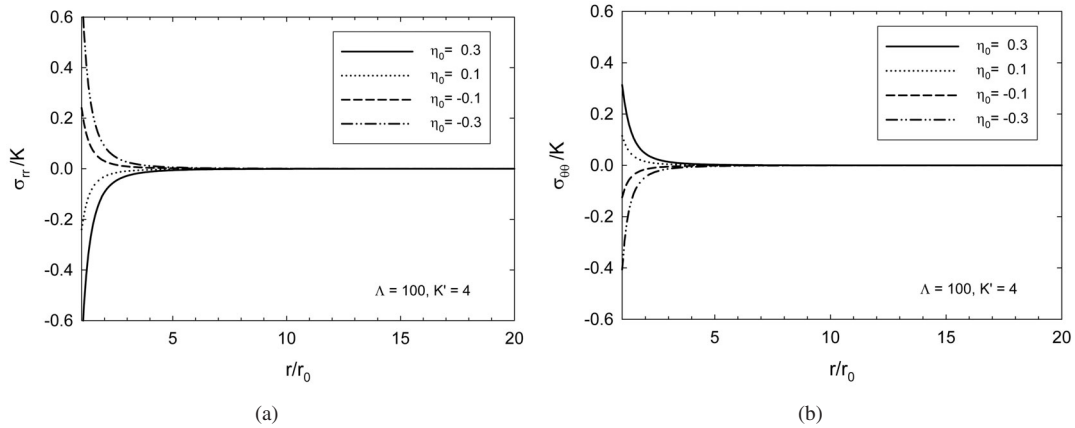


Fig. 5 Cauchy stress for point defect with $K' = 4$ and $\Lambda = 100$: (a) radial stress (b) circumferential stress.

and Fig. 4(d) for $\eta_0 = 0.3$ and $\eta_0 = -0.3$: for $\Lambda \geq 100$, radial displacements are indistinguishable. For $\Lambda \leq 10$, increased magnitudes of u are observed since the unconstrained surface at R_0 is closer to the core.

Normalized Cauchy stress field σ/K is shown in Fig. 5 for $\Lambda = 100$ and $K' = 4$. Radial stress σ_{rr} is shown in Fig. 5(a), circumferential $\sigma_{\theta\theta} = \sigma_{\phi\phi}$ in Fig. 5(b). Maximum magnitudes at $r = r_0$ are on the order of $K/2$. Radial and circumferential stress components are of opposite sign and decay rapidly within $r \lesssim 10r_0$.

Nonlinear and linear solutions for stress and normalized volume change are compared in Fig. 6 and Table 2, respectively. Stress components shown in Fig. 6 correspond to fixed parameters $\Lambda = 100, \eta_0 = -0.3$ (linear and nonlinear) and

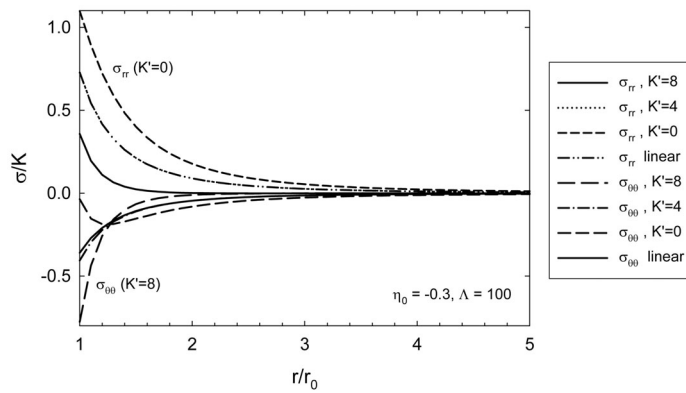


Fig. 6 Nonlinear and linear elastic solutions for stress field of point defect with $\Lambda = 100$ and $\eta_0 = -0.3$.

$K' = 0, 4, 8$ (nonlinear). For $K' = 4$, stresses obtained from the nonlinear solution are almost indistinguishable from corresponding stresses of the linear solution. For $K' \neq 4$, differences among stress predictions are evident near the core, e.g., for $r \lesssim 5r_0$. Solutions for normalized volume change in Table 2 are obtained using (5.47). The linear solution [14, 81] is $\Delta V/\delta v = 3(1 - \nu)/(1 + \nu)$; this yields a value of $\frac{9}{5}$ when $\nu = \frac{1}{4}$. As shown in Table 2, volume change is strongly affected by elastic nonlinearity. For a material with K' differing substantially from 4, nonlinear theory should be used to predict volume change from point defects, even though stress components may not differ significantly between linear and nonlinear solutions for $r \gtrsim 5r_0$.

Table 2 Volume change $\Delta V/\delta v$ for point defect, $\Lambda = 100$.

η_0	$K' = 0$	$K' = 2$	$K' = 4$	$K' = 6$	$K' = 8$	linear
0.3	0.00	0.93	1.85	2.78	3.70	1.80
0.1	1.20	1.51	1.82	2.13	2.43	1.80
-0.1	2.40	2.09	1.78	1.47	1.17	1.80
-0.3	3.60	2.67	1.75	0.82	-0.10	1.80

6 Conclusions

A nonlinear differential geometric framework of defective crystals has been presented, incorporating a multiplicative decomposition of the deformation gradient into up to three terms and an additive decomposition of a linear connection describing covariant derivatives of a field of lattice director vectors. This theoretical framework has been applied to describe three different singular defects: the screw dislocation, the wedge disclination, and the point defect. Inelastic deformation is quantified for each defect using generalized functions in the sense of Gel'fand and Shilov, wherein singular parts of the deformation gradient are defined as inelastic. This particular application of the multiplicative decomposition of the deformation gradient for singular defects in the nonlinear theory is original. Analytical second-order solutions have been obtained in the context of isotropic compressible nonlinear elasticity. These solutions are all new, incorporating an elastic potential depending on an Eulerian strain measure in material coordinates with elastic constants up to third order. The iterative solution procedure used herein omits, in the stress components, products of orders three and higher in certain strain gradient components. Thus the present solutions are expected to be reasonably accurate when such higher-order products are small, though exact solutions are not available for comparison. For the screw dislocation, radial displacements and dilatation are strongly affected by elastic nonlinearity and core pressure, while stress fields tend to converge to linear elastic solutions within a radial distance of 10–20 lattice parameters from the core. For the wedge disclination, effects of core pressure on radial displacement and stress fields that have not been presented in previous linear or nonlinear analyses are included. For the point defect, radial displacement and stress decay rapidly with distance from the core, but total volume change in the body due to the point defect depends strongly on elastic nonlinearity.

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Appendix A: cylindrical coordinates

Reference cylindrical coordinates $\{X^A\}$ are

$$(X^1, X^2, X^3) = (R, \Theta, Z). \quad (\text{A.1})$$

Let \mathbf{X} denote the position vector measured from the fixed origin:

$$\mathbf{X}(R, \Theta, Z) = R\mathbf{G}_R + Z\mathbf{G}_Z. \quad (\text{A.2})$$

Natural basis vectors are

$$\mathbf{G}_A = \partial_A \mathbf{X}; \quad \mathbf{G}_R(\Theta) = \partial_R \mathbf{X}, \quad \mathbf{G}_\Theta(R, \Theta) = \partial_\Theta \mathbf{X}, \quad \mathbf{G}_Z = \partial_Z \mathbf{X}. \quad (\text{A.3})$$

The metric tensor with components $G_{AB} = \mathbf{G}_A \cdot \mathbf{G}_B$ and its inverse are

$$[G_{AB}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & R^2 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad [G^{AB}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1/R^2 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (\text{A.4})$$

Contravariant basis vectors are

$$\mathbf{G}^A = G^{AB} \mathbf{G}_B; \quad \mathbf{G}^R(\Theta) = \mathbf{G}_R, \quad \mathbf{G}^\Theta(R, \Theta) = (1/R^2)\mathbf{G}_\Theta, \quad \mathbf{G}^Z = \mathbf{G}_Z. \quad (\text{A.5})$$

Physical (dimensionless unit) basis vectors are

$$\mathbf{E}_A = \mathbf{G}_A / \sqrt{G_{AA}}; \quad \mathbf{E}_R(\Theta) = \mathbf{G}_R, \quad \mathbf{E}_\Theta(\Theta) = (1/R)\mathbf{G}_\Theta, \quad \mathbf{E}_Z = \mathbf{G}_Z. \quad (\text{A.6})$$

Since cylindrical coordinates are orthogonal ($\mathbf{E}_A = \mathbf{E}^A$), there is no need to distinguish between contravariant and covariant physical components. Cylindrical coordinates are related to Cartesian coordinates as follows:

$$X = R \cos \Theta, \quad Y = R \sin \Theta; \quad \mathbf{X} = X\mathbf{E}_X + Y\mathbf{E}_Y + Z\mathbf{E}_Z; \quad (\text{A.7})$$

$$\mathbf{E}_R = \cos \Theta \mathbf{E}_X + \sin \Theta \mathbf{E}_Y, \quad \mathbf{E}_\Theta = -\sin \Theta \mathbf{E}_X + \cos \Theta \mathbf{E}_Y, \quad \mathbf{E}_Z = \mathbf{E}_Z. \quad (\text{A.8})$$

Spatial cylindrical coordinate chart $\{x^a\}$ has coordinates

$$(x^1, x^2, x^3) = (r, \theta, z). \quad (\text{A.9})$$

Let \mathbf{x} denote the position vector measured from the fixed origin:

$$\mathbf{x}(r, \theta, z) = r\mathbf{g}_r + z\mathbf{g}_z. \quad (\text{A.10})$$

Natural basis vectors are

$$\mathbf{g}_a = \partial_a \mathbf{x}; \quad \mathbf{g}_r(\theta) = \partial_r \mathbf{x}, \quad \mathbf{g}_\theta(r, \theta) = \partial_\theta \mathbf{x}, \quad \mathbf{g}_z = \partial_z \mathbf{x}. \quad (\text{A.11})$$

The metric tensor with components $g_{ab} = \mathbf{g}_a \cdot \mathbf{g}_b$ and its inverse are

$$[g_{ab}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad [g^{ab}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1/r^2 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (\text{A.12})$$

Contravariant basis vectors are

$$\mathbf{g}^a = g^{ab} \mathbf{g}_b; \quad \mathbf{g}^r(\theta) = \mathbf{g}_r, \quad \mathbf{g}^\theta(r, \theta) = (1/r^2) \mathbf{g}_\theta, \quad \mathbf{g}^z = \mathbf{g}_z. \quad (\text{A.13})$$

Physical basis vectors are

$$\mathbf{e}_a = \mathbf{g}_a / \sqrt{g_{aa}}; \quad \mathbf{e}_r(\theta) = \mathbf{g}_r, \quad \mathbf{e}_\theta(\theta) = (1/r) \mathbf{g}_\theta, \quad \mathbf{e}_z = \mathbf{g}_z. \quad (\text{A.14})$$

Cylindrical coordinates are related to Cartesian coordinates as

$$x = r \cos \theta, \quad y = r \sin \theta; \quad \mathbf{x} = x \mathbf{e}_x + y \mathbf{e}_y + z \mathbf{e}_z; \quad (\text{A.15})$$

$$\mathbf{e}_r = \cos \theta \mathbf{e}_x + \sin \theta \mathbf{e}_y, \quad \mathbf{e}_\theta = -\sin \theta \mathbf{e}_x + \cos \theta \mathbf{e}_y, \quad \mathbf{e}_z = \mathbf{e}_z. \quad (\text{A.16})$$

In this paper, coincident Cartesian frames are used such that $\mathbf{E}_A = \delta_A^a \mathbf{e}_a$:

$$\mathbf{E}_X = \mathbf{e}_x, \quad \mathbf{E}_Y = \mathbf{e}_y, \quad \mathbf{E}_Z = \mathbf{e}_z. \quad (\text{A.17})$$

Mixed variant components of the shifter tensor between reference and spatial systems are [14, 15, 35]

$$g_A^a(\mathbf{x}, \mathbf{X}) = \langle \mathbf{g}^a, \mathbf{G}_A \rangle; \quad \mathbf{g}^a(\mathbf{x}) = g_A^a \mathbf{G}^A(\mathbf{X}); \quad (\text{A.18})$$

where $\langle \cdot, \cdot \rangle$ denotes a scalar product. Using (A.17), it follows that

$$\begin{aligned} g_R^r(\theta, \Theta) &= \langle \mathbf{g}^r(\theta), \mathbf{G}_R(\Theta) \rangle = \mathbf{e}_r(\theta) \cdot \mathbf{E}_R(\Theta) \\ &= (\cos \theta \mathbf{e}_x + \sin \theta \mathbf{e}_y) \cdot (\cos \Theta \mathbf{E}_X + \sin \Theta \mathbf{E}_Y) = \cos(\theta - \Theta). \end{aligned} \quad (\text{A.19})$$

Applying similar calculations, the matrix of components of $g_A^a(r, \theta; R, \Theta)$ is

$$[g_A^a] = \begin{bmatrix} g_R^r & g_\Theta^r & g_Z^r \\ g_R^\theta & g_\Theta^\theta & g_Z^\theta \\ g_R^z & g_\Theta^z & g_Z^z \end{bmatrix} = \begin{bmatrix} \cos(\theta - \Theta) & R \sin(\theta - \Theta) & 0 \\ -(1/r) \sin(\theta - \Theta) & (R/r) \cos(\theta - \Theta) & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (\text{A.20})$$

The inverse of $[g_A^a]$ is $[g_a^A]$, such that $g_A^a g_b^A = \delta_b^a$:

$$[g_a^A] = \begin{bmatrix} g_r^R & g_\theta^R & g_z^R \\ g_r^\Theta & g_\theta^\Theta & g_z^\Theta \\ g_r^Z & g_\theta^Z & g_z^Z \end{bmatrix} = \begin{bmatrix} \cos(\theta - \Theta) & -r \sin(\theta - \Theta) & 0 \\ (1/R) \sin(\theta - \Theta) & (r/R) \cos(\theta - \Theta) & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (\text{A.21})$$

Letting $G = \det[G_{AB}]$ and $g = \det[g_{ab}]$, determinants obey

$$\det[g_A^a] = \sqrt{G/g} = R/r, \quad \det[g_a^A] = \sqrt{g/G} = r/R. \quad (\text{A.22})$$

In cylindrical coordinates, deformation $\mathbf{x} = \mathbf{x}(\mathbf{X})$ is of the form

$$r = r(R, \Theta, Z), \quad \theta = \theta(R, \Theta, Z), \quad z = z(R, \Theta, Z). \quad (\text{A.23})$$

Referred to natural bases $\{\mathbf{g}_a, \mathbf{G}^A\}$, the deformation gradient is

$$\begin{aligned} \mathbf{F} &= \partial_A \mathbf{x} \otimes \mathbf{G}^A = \partial_A x^a \mathbf{g}_a \otimes \mathbf{G}^A = F_{iA}^a \mathbf{g}_a \otimes \mathbf{G}^A \\ &= \partial_R r \mathbf{g}_r \otimes \mathbf{G}^R + \partial_\Theta r \mathbf{g}_r \otimes \mathbf{G}^\Theta + \partial_Z r \mathbf{g}_r \otimes \mathbf{G}^Z \\ &\quad + \partial_R \theta \mathbf{g}_\theta \otimes \mathbf{G}^R + \partial_\Theta \theta \mathbf{g}_\theta \otimes \mathbf{G}^\Theta + \partial_Z \theta \mathbf{g}_\theta \otimes \mathbf{G}^Z \\ &\quad + \partial_R z \mathbf{g}_z \otimes \mathbf{G}^R + \partial_\Theta z \mathbf{g}_z \otimes \mathbf{G}^\Theta + \partial_Z z \mathbf{g}_z \otimes \mathbf{G}^Z. \end{aligned} \quad (\text{A.24})$$

Referential and deformed volume elements

$$dV = \sqrt{G} dX^1 dX^2 dX^3 = R dR d\Theta dZ, \quad dv = \sqrt{g} dx^1 dx^2 dx^3 = r dr d\theta dz \quad (\text{A.25})$$

are related through the Jacobian determinant

$$J = dv/dV = \det[F_{,A}^a] \sqrt{g/G} = \det[\partial_A x^a] \det[g_a^A] = \det[\partial_A x^a] (r/R). \quad (\text{A.26})$$

Using (A.5), (A.6), and (A.14) to convert natural bases to orthonormal bases $\{\mathbf{e}_a, \mathbf{E}_A\}$, the two-point deformation gradient in physical components is

$$\begin{aligned} \mathbf{F} &= F_{\langle aA \rangle} \mathbf{e}_a \otimes \mathbf{E}_A \\ &= \partial_R r \mathbf{e}_r \otimes \mathbf{E}_R + (1/R) \partial_\Theta r \mathbf{e}_r \otimes \mathbf{E}_\Theta + \partial_Z r \mathbf{e}_r \otimes \mathbf{E}_Z \\ &\quad + r \partial_R \theta \mathbf{e}_\theta \otimes \mathbf{E}_R + (r/R) \partial_\Theta \theta \mathbf{e}_\theta \otimes \mathbf{E}_\Theta + r \partial_Z \theta \mathbf{e}_\theta \otimes \mathbf{E}_Z \\ &\quad + \partial_R z \mathbf{e}_z \otimes \mathbf{E}_R + (1/R) \partial_\Theta z \mathbf{e}_z \otimes \mathbf{E}_\Theta + \partial_Z z \mathbf{e}_z \otimes \mathbf{E}_Z, \end{aligned} \quad (\text{A.27})$$

where physical scalar components are written in angled brackets. The Jacobian is

$$J = \det[F_{\langle aA \rangle}]. \quad (\text{A.28})$$

Using the shifter (A.21), the deformation gradient can be expressed completely with respect to Lagrangian bases:

$$\begin{aligned} \mathbf{F} &= \partial_A x^a (g_a^B \mathbf{G}_B) \otimes \mathbf{G}^A = [\partial_A x^a g_a^B] \mathbf{G}_B \otimes \mathbf{G}^A \\ &= [\partial_R r \cos(\theta - \Theta) - r \partial_R \theta \sin(\theta - \Theta)] \mathbf{G}_R \otimes \mathbf{G}^R \\ &\quad + [\partial_\Theta r \cos(\theta - \Theta) - r \partial_\Theta \theta \sin(\theta - \Theta)] \mathbf{G}_R \otimes \mathbf{G}^\Theta \\ &\quad + [\partial_Z r \cos(\theta - \Theta) - r \partial_Z \theta \sin(\theta - \Theta)] \mathbf{G}_R \otimes \mathbf{G}^Z \\ &\quad + [(1/R) \partial_R r \sin(\theta - \Theta) + (r/R) \partial_R \theta \cos(\theta - \Theta)] \mathbf{G}_\Theta \otimes \mathbf{G}^R \\ &\quad + [(1/R) \partial_\Theta r \sin(\theta - \Theta) + (r/R) \partial_\Theta \theta \cos(\theta - \Theta)] \mathbf{G}_\Theta \otimes \mathbf{G}^\Theta \\ &\quad + [(1/R) \partial_Z r \sin(\theta - \Theta) + (r/R) \partial_Z \theta \cos(\theta - \Theta)] \mathbf{G}_\Theta \otimes \mathbf{G}^Z \\ &\quad + [\partial_R z] \mathbf{G}_Z \otimes \mathbf{G}^R + [\partial_\Theta z] \mathbf{G}_Z \otimes \mathbf{G}^\Theta + [\partial_Z z] \mathbf{G}_Z \otimes \mathbf{G}^Z. \end{aligned} \quad (\text{A.29})$$

In physical components this becomes

$$\begin{aligned} \mathbf{F} &= F_{\langle AB \rangle} \mathbf{E}_A \otimes \mathbf{E}_B \\ &= [\partial_R r \cos(\theta - \Theta) - r \partial_R \theta \sin(\theta - \Theta)] \mathbf{E}_R \otimes \mathbf{E}_R \\ &\quad + [(1/R) \partial_\Theta r \cos(\theta - \Theta) - (r/R) \partial_\Theta \theta \sin(\theta - \Theta)] \mathbf{E}_R \otimes \mathbf{E}_\Theta \\ &\quad + [\partial_Z r \cos(\theta - \Theta) - r \partial_Z \theta \sin(\theta - \Theta)] \mathbf{E}_R \otimes \mathbf{E}_Z \\ &\quad + [\partial_R r \sin(\theta - \Theta) + r \partial_R \theta \cos(\theta - \Theta)] \mathbf{E}_\Theta \otimes \mathbf{E}_R \\ &\quad + [(1/R) \partial_\Theta r \sin(\theta - \Theta) + (r/R) \partial_\Theta \theta \cos(\theta - \Theta)] \mathbf{E}_\Theta \otimes \mathbf{E}_\Theta \\ &\quad + [\partial_Z r \sin(\theta - \Theta) + r \partial_Z \theta \cos(\theta - \Theta)] \mathbf{E}_\Theta \otimes \mathbf{E}_Z \\ &\quad + [\partial_R z] \mathbf{E}_Z \otimes \mathbf{E}_R + [(1/R) \partial_\Theta z] \mathbf{E}_Z \otimes \mathbf{E}_\Theta + [\partial_Z z] \mathbf{E}_Z \otimes \mathbf{E}_Z. \end{aligned} \quad (\text{A.30})$$

Similarly, expressing \mathbf{F} entirely with respect to natural spatial bases,

$$\begin{aligned} \mathbf{F} &= \partial_A x^a \mathbf{g}_a \otimes (g_b^A \mathbf{g}^b) = [\partial_A x^a g_b^A] \mathbf{g}_a \otimes \mathbf{g}^b \\ &= [\partial_R r \cos(\theta - \Theta) + (1/R) \partial_\Theta r \sin(\theta - \Theta)] \mathbf{g}_r \otimes \mathbf{g}^r \\ &\quad + [\partial_R \theta \cos(\theta - \Theta) + (1/R) \partial_\Theta \theta \sin(\theta - \Theta)] \mathbf{g}_\theta \otimes \mathbf{g}^r \\ &\quad + [\partial_R z \cos(\theta - \Theta) + (1/R) \partial_\Theta z \sin(\theta - \Theta)] \mathbf{g}_z \otimes \mathbf{g}^r \\ &\quad + [-r \partial_R r \sin(\theta - \Theta) + (r/R) \partial_\Theta r \cos(\theta - \Theta)] \mathbf{g}_r \otimes \mathbf{g}^\theta \\ &\quad + [-r \partial_R \theta \sin(\theta - \Theta) + (r/R) \partial_\Theta \theta \cos(\theta - \Theta)] \mathbf{g}_\theta \otimes \mathbf{g}^\theta \\ &\quad + [-r \partial_R z \sin(\theta - \Theta) + (r/R) \partial_\Theta z \cos(\theta - \Theta)] \mathbf{g}_z \otimes \mathbf{g}^\theta \\ &\quad + [\partial_Z r] \mathbf{g}_r \otimes \mathbf{g}^z + [\partial_Z \theta] \mathbf{g}_\theta \otimes \mathbf{g}^z + [\partial_Z z] \mathbf{g}_z \otimes \mathbf{g}^z. \end{aligned} \quad (\text{A.31})$$

In spatial physical components,

$$\begin{aligned}
\mathbf{F} &= F_{\langle ab \rangle} \mathbf{e}_a \otimes \mathbf{e}_b \\
&= [\partial_R r \cos(\theta - \Theta) + (1/R) \partial_\Theta r \sin(\theta - \Theta)] \mathbf{e}_r \otimes \mathbf{e}_r \\
&\quad + [r \partial_R \theta \cos(\theta - \Theta) + (r/R) \partial_\Theta \theta \sin(\theta - \Theta)] \mathbf{e}_\theta \otimes \mathbf{e}_r \\
&\quad + [\partial_R z \cos(\theta - \Theta) + (1/R) \partial_\Theta z \sin(\theta - \Theta)] \mathbf{e}_z \otimes \mathbf{e}_r \\
&\quad + [-\partial_R r \sin(\theta - \Theta) + (1/R) \partial_\Theta r \cos(\theta - \Theta)] \mathbf{e}_r \otimes \mathbf{e}_\theta \\
&\quad + [-r \partial_R \theta \sin(\theta - \Theta) + (r/R) \partial_\Theta \theta \cos(\theta - \Theta)] \mathbf{e}_\theta \otimes \mathbf{e}_\theta \\
&\quad + [-\partial_R z \sin(\theta - \Theta) + (1/R) \partial_\Theta z \cos(\theta - \Theta)] \mathbf{e}_z \otimes \mathbf{e}_\theta \\
&\quad + [\partial_Z r] \mathbf{e}_r \otimes \mathbf{e}_z + [r \partial_Z \theta] \mathbf{e}_\theta \otimes \mathbf{e}_z + [\partial_Z z] \mathbf{e}_z \otimes \mathbf{e}_z.
\end{aligned} \tag{A.32}$$

Letting $\mathbf{F} \rightarrow \mathbf{F}^P$, (A.29) becomes an example of the plastic deformation gradient referred to coincident curvilinear coordinate frames in reference and intermediate configurations, as used in [14, 15, 18, 75]. With $\mathbf{F} \rightarrow \mathbf{F}^L$, (A.31) becomes an example of coincident curvilinear systems in current and intermediate configurations, as in [14, 15].

In cylindrical coordinates, inverse deformation $\mathbf{X} = \mathbf{X}(\mathbf{x})$ is of the form

$$R = R(r, \theta, z), \quad \Theta = \Theta(r, \theta, z), \quad Z = Z(r, \theta, z). \tag{A.33}$$

Referred to natural bases $\{\mathbf{G}_A, \mathbf{g}^a\}$, the inverse deformation gradient is

$$\begin{aligned}
\mathbf{F}^{-1} &= \partial_a \mathbf{X} \otimes \mathbf{g}^a = \partial_a X^A \mathbf{G}_A \otimes \mathbf{g}^a = F^{-1A}{}_{,a} \mathbf{G}_A \otimes \mathbf{g}^a \\
&= \partial_r R \mathbf{G}_R \otimes \mathbf{g}^r + \partial_\theta R \mathbf{G}_R \otimes \mathbf{g}^\theta + \partial_z R \mathbf{G}_R \otimes \mathbf{g}^z \\
&\quad + \partial_r \Theta \mathbf{G}_\Theta \otimes \mathbf{g}^r + \partial_\theta \Theta \mathbf{G}_\Theta \otimes \mathbf{g}^\theta + \partial_z \Theta \mathbf{G}_\Theta \otimes \mathbf{g}^z \\
&\quad + \partial_r Z \mathbf{G}_Z \otimes \mathbf{g}^r + \partial_\theta Z \mathbf{G}_Z \otimes \mathbf{g}^\theta + \partial_z Z \mathbf{G}_Z \otimes \mathbf{g}^z.
\end{aligned} \tag{A.34}$$

The inverse of the Jacobian determinant $J^{-1} = 1/J$ is

$$J^{-1} = dV/dv = \det[F^{-1A}{}_{,a}] \sqrt{G/g} = \det[\partial_a X^A] \det[g_a^A] = \det[\partial_a X^A] (R/r). \tag{A.35}$$

In orthonormal bases $\{\mathbf{E}_A, \mathbf{e}_a\}$, two-point inverse deformation gradient is

$$\begin{aligned}
\mathbf{F}^{-1} &= F_{\langle Aa \rangle}^{-1} \mathbf{E}_A \otimes \mathbf{e}_a \\
&= \partial_r R \mathbf{E}_R \otimes \mathbf{e}_r + (1/r) \partial_\theta R \mathbf{E}_R \otimes \mathbf{e}_\theta + \partial_z R \mathbf{E}_R \otimes \mathbf{e}_z \\
&\quad + R \partial_r \Theta \mathbf{E}_\Theta \otimes \mathbf{e}_r + (R/r) \partial_\theta \Theta \mathbf{E}_\Theta \otimes \mathbf{e}_\theta + R \partial_z \Theta \mathbf{E}_\Theta \otimes \mathbf{e}_z \\
&\quad + \partial_r Z \mathbf{E}_Z \otimes \mathbf{e}_r + (1/r) \partial_\theta Z \mathbf{E}_Z \otimes \mathbf{e}_\theta + \partial_z Z \mathbf{E}_Z \otimes \mathbf{e}_z,
\end{aligned} \tag{A.36}$$

with inverse Jacobian determinant

$$J^{-1} = \det[F_{\langle Aa \rangle}^{-1}]. \tag{A.37}$$

A spatial displacement field in physical cylindrical coordinates can be constructed using the shifter:

$$\begin{aligned}
\mathbf{u} &= \mathbf{x} - \mathbf{X} = r \mathbf{g}_r + z \mathbf{g}_z - R \mathbf{G}_R - Z \mathbf{G}_Z = r \mathbf{g}_r - R g_R^a \mathbf{g}_a + (z - Z) \mathbf{G}_Z \\
&= [r - R \cos(\theta - \Theta)] \mathbf{e}_r + [R \sin(\theta - \Theta)] \mathbf{e}_\theta + [z - Z] \mathbf{e}_z = u_r \mathbf{e}_r + u_\theta \mathbf{e}_\theta + u_z \mathbf{e}_z.
\end{aligned} \tag{A.38}$$

The divergence of a second-order tensor field $\mathbf{A}(\mathbf{x}) = A_{\langle ab \rangle} \mathbf{e}_a \otimes \mathbf{e}_b$ is, in physical cylindrical coordinates [65],

$$\begin{aligned}
\nabla \cdot \mathbf{A} &= [(1/r) \partial_r (r A_{rr}) + (1/r) \partial_\theta A_{\theta r} + \partial_z A_{zr} - (1/r) A_{\theta\theta}] \mathbf{e}_r \\
&\quad + [(1/r) \partial_r (r A_{r\theta}) + (1/r) \partial_\theta A_{\theta\theta} + \partial_z A_{z\theta} + (1/r) A_{\theta r}] \mathbf{e}_\theta \\
&\quad + [(1/r) \partial_r (r A_{rz}) + (1/r) \partial_\theta A_{\theta z} + \partial_z A_{zz}] \mathbf{e}_z.
\end{aligned} \tag{A.39}$$

Appendix B: spherical coordinates

Reference spherical coordinates $\{X^A\}$ are

$$(X^1, X^2, X^3) = (R, \Theta, \Phi). \quad (\text{B.1})$$

Let \mathbf{X} denote the position vector measured from a fixed origin:

$$\mathbf{X}(R, \Theta, \Phi) = R\mathbf{G}_R(\Theta, \Phi). \quad (\text{B.2})$$

Natural basis vectors are

$$\mathbf{G}_A = \partial_A \mathbf{X}; \quad \mathbf{G}_R(\Theta, \Phi) = \partial_R \mathbf{X}, \quad \mathbf{G}_\Theta(R, \Theta, \Phi) = \partial_\Theta \mathbf{X}, \quad \mathbf{G}_\Phi(R, \Theta, \Phi) = \partial_\Phi \mathbf{X}. \quad (\text{B.3})$$

The metric tensor with components $G_{AB} = \mathbf{G}_A \cdot \mathbf{G}_B$ and its inverse are

$$[G_{AB}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & R^2 & 0 \\ 0 & 0 & R^2 \sin^2 \Theta \end{bmatrix}, \quad [G^{AB}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1/R^2 & 0 \\ 0 & 0 & 1/(R^2 \sin^2 \Theta) \end{bmatrix}. \quad (\text{B.4})$$

Contravariant basis vectors are

$$\mathbf{G}^A = G^{AB} \mathbf{G}_B; \quad \mathbf{G}^R = \mathbf{G}_R, \quad \mathbf{G}^\Theta = (1/R^2) \mathbf{G}_\Theta, \quad \mathbf{G}^\Phi = [1/(R^2 \sin^2 \Theta)] \mathbf{G}_\Phi. \quad (\text{B.5})$$

Physical (dimensionless unit) basis vectors are

$$\mathbf{E}_A = \mathbf{G}_A / \sqrt{G_{AA}}; \quad \mathbf{E}_R = \mathbf{G}_R, \quad \mathbf{E}_\Theta = (1/R) \mathbf{G}_\Theta, \quad \mathbf{E}_\Phi = [1/(R \sin \Theta)] \mathbf{G}_\Phi. \quad (\text{B.6})$$

Since spherical coordinates are orthogonal ($\mathbf{E}_A = \mathbf{E}^A$), there is no need to distinguish between contravariant and covariant physical components. Spherical coordinates are related to Cartesian coordinates as follows:

$$X = R \sin \Theta \cos \Phi, \quad Y = R \sin \Theta \sin \Phi, \quad Z = R \cos \Theta; \quad \mathbf{X} = X \mathbf{E}_X + Y \mathbf{E}_Y + Z \mathbf{E}_Z; \quad (\text{B.7})$$

$$\begin{aligned} \mathbf{E}_R &= \sin \Theta \cos \Phi \mathbf{E}_X + \sin \Theta \sin \Phi \mathbf{E}_Y + \cos \Theta \mathbf{E}_Z, \\ \mathbf{E}_\Theta &= \cos \Theta \cos \Phi \mathbf{E}_X + \cos \Theta \sin \Phi \mathbf{E}_Y - \sin \Theta \mathbf{E}_Z, \\ \mathbf{E}_\Phi &= -\sin \Phi \mathbf{E}_X + \cos \Phi \mathbf{E}_Y. \end{aligned} \quad (\text{B.8})$$

Spatial spherical coordinate chart $\{x^a\}$ has coordinates

$$(x^1, x^2, x^3) = (r, \theta, \phi). \quad (\text{B.9})$$

Let \mathbf{x} denote the position vector measured from a fixed origin:

$$\mathbf{x}(r, \theta, \phi) = r \mathbf{g}_r(\theta, \phi). \quad (\text{B.10})$$

Natural basis vectors are

$$\mathbf{g}_a = \partial_a \mathbf{x}; \quad \mathbf{g}_r(\theta, \phi) = \partial_r \mathbf{x}, \quad \mathbf{g}_\theta(r, \theta, \phi) = \partial_\theta \mathbf{x}, \quad \mathbf{g}_\phi(r, \theta, \phi) = \partial_\phi \mathbf{x}. \quad (\text{B.11})$$

The metric tensor with components $g_{ab} = \mathbf{g}_a \cdot \mathbf{g}_b$ and its inverse are

$$[g_{ab}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & r^2 \sin^2 \phi \end{bmatrix}, \quad [g^{ab}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1/r^2 & 0 \\ 0 & 0 & 1/(r^2 \sin^2 \phi) \end{bmatrix}. \quad (\text{B.12})$$

Contravariant basis vectors are

$$\mathbf{g}^a = g^{ab} \mathbf{g}_b; \quad \mathbf{g}^r = \mathbf{g}_r, \quad \mathbf{g}^\theta = (1/r^2) \mathbf{g}_\theta, \quad \mathbf{g}^\phi = [1/(r^2 \sin^2 \theta)] \mathbf{g}_\phi. \quad (\text{B.13})$$

Physical basis vectors are

$$\mathbf{e}_a = \mathbf{g}_a / \sqrt{g_{aa}}; \quad \mathbf{e}_r = \mathbf{g}_r, \quad \mathbf{e}_\theta = (1/r)\mathbf{g}_\theta, \quad \mathbf{e}_\phi = [1/(r \sin \theta)]\mathbf{g}_\phi. \quad (\text{B.14})$$

Spherical coordinates are related to Cartesian coordinates as

$$x = r \sin \theta \cos \phi, \quad y = r \sin \theta \sin \phi, \quad z = r \cos \theta; \quad \mathbf{x} = x\mathbf{e}_x + y\mathbf{e}_y + z\mathbf{e}_z; \quad (\text{B.15})$$

$$\begin{aligned} \mathbf{e}_r &= \sin \theta \cos \phi \mathbf{e}_x + \sin \theta \sin \phi \mathbf{e}_y + \cos \theta \mathbf{e}_z, \\ \mathbf{e}_\theta &= \cos \theta \cos \phi \mathbf{e}_x + \cos \theta \sin \phi \mathbf{e}_y - \sin \theta \mathbf{e}_z, \\ \mathbf{e}_\phi &= -\sin \phi \mathbf{e}_x + \cos \phi \mathbf{e}_y. \end{aligned} \quad (\text{B.16})$$

Using (A.17), the matrix of shifter components $g_A^a(r, \theta, \phi; R, \Theta, \Phi)$ is

$$[g_A^a] = \begin{bmatrix} g_R^r & g_\Theta^r & g_\Phi^r \\ g_R^\theta & g_\Theta^\theta & g_\Phi^\theta \\ g_R^\phi & g_\Theta^\phi & g_\Phi^\phi \end{bmatrix}; \quad (\text{B.17})$$

$$g_R^r = \sin \theta \sin \Theta \cos(\phi - \Phi) + \cos \theta \cos \Theta, \quad (\text{B.18})$$

$$g_\Theta^r = R[\sin \theta \cos \Theta \cos(\phi - \Phi) - \cos \theta \sin \Theta], \quad (\text{B.19})$$

$$g_\Phi^r = R \sin \theta \sin \Theta \sin(\phi - \Phi), \quad (\text{B.20})$$

$$g_R^\theta = (1/r)[\cos \theta \sin \Theta \cos(\phi - \Phi) - \sin \theta \cos \Theta], \quad (\text{B.21})$$

$$g_\Theta^\theta = (R/r)[\cos \theta \cos \Theta \cos(\phi - \Phi) + \sin \theta \sin \Theta], \quad (\text{B.22})$$

$$g_\Phi^\theta = (R/r) \cos \theta \sin \Theta \sin(\phi - \Phi), \quad (\text{B.23})$$

$$g_R^\phi = -[\sin \Theta / (r \sin \theta)] \sin(\phi - \Phi), \quad (\text{B.24})$$

$$g_\Theta^\phi = -[(R \cos \Theta) / (r \sin \theta)] \sin(\phi - \Phi), \quad (\text{B.25})$$

$$g_\Phi^\phi = [(R \sin \Theta) / (r \sin \theta)] \cos(\phi - \Phi). \quad (\text{B.26})$$

Letting $G = \det[G_{AB}] = R^4 \sin^2 \Theta$ and $g = \det[g_{ab}] = r^4 \sin^2 \theta$, determinants obey

$$\det[g_A^a] = \sqrt{G/g} = R^2 \sin \Theta / (r^2 \sin \theta), \quad \det[g_a^A] = \sqrt{g/G} = r^2 \sin \theta / (R^2 \sin \Theta). \quad (\text{B.27})$$

In spherical coordinates, deformation $\mathbf{x} = \mathbf{x}(\mathbf{X})$ is of the form

$$r = r(R, \Theta, \Phi), \quad \theta = \theta(R, \Theta, \Phi), \quad \phi = \phi(R, \Theta, \Phi). \quad (\text{B.28})$$

Referred to natural bases $\{\mathbf{g}_a, \mathbf{G}^A\}$, the deformation gradient is

$$\begin{aligned} \mathbf{F} &= \partial_A \mathbf{x} \otimes \mathbf{G}^A = \partial_A x^a \mathbf{g}_a \otimes \mathbf{G}^A = F_{,A}^a \mathbf{g}_a \otimes \mathbf{G}^A \\ &= \partial_R r \mathbf{g}_r \otimes \mathbf{G}^R + \partial_\Theta r \mathbf{g}_r \otimes \mathbf{G}^\Theta + \partial_\Phi r \mathbf{g}_r \otimes \mathbf{G}^\Phi \\ &\quad + \partial_R \theta \mathbf{g}_\theta \otimes \mathbf{G}^R + \partial_\Theta \theta \mathbf{g}_\theta \otimes \mathbf{G}^\Theta + \partial_\Phi \theta \mathbf{g}_\theta \otimes \mathbf{G}^\Phi \\ &\quad + \partial_R \phi \mathbf{g}_\phi \otimes \mathbf{G}^R + \partial_\Theta \phi \mathbf{g}_\phi \otimes \mathbf{G}^\Theta + \partial_\Phi \phi \mathbf{g}_\phi \otimes \mathbf{G}^\Phi. \end{aligned} \quad (\text{B.29})$$

Referential and deformed volume elements

$$dV = \sqrt{G} dX^1 dX^2 dX^3 = R^2 \sin \Theta dR d\Theta d\Phi, \quad dv = \sqrt{g} dx^1 dx^2 dx^3 = r^2 \sin \theta dr d\theta d\phi \quad (\text{B.30})$$

are related through the Jacobian determinant

$$J = dv/dV = \det[F_{,A}^a] \sqrt{g/G} = \det[\partial_A x^a] \det[g_a^A] = \det[\partial_A x^a] [r^2 \sin \theta / (R^2 \sin \Theta)]. \quad (\text{B.31})$$

Using (B.5), (B.6), and (B.14) to convert natural basis vectors to spherical orthonormal bases $\{\mathbf{e}_a, \mathbf{E}_A\}$, the two-point deformation gradient in physical components is

$$\begin{aligned} \mathbf{F} &= F_{\langle aA \rangle} \mathbf{e}_a \otimes \mathbf{E}_A \\ &= \partial_R r \mathbf{e}_r \otimes \mathbf{E}_R + (1/R) \partial_\Theta r \mathbf{e}_r \otimes \mathbf{E}_\Theta + [1/(R \sin \Theta)] \partial_\Phi r \mathbf{e}_r \otimes \mathbf{E}_\Phi \\ &\quad + r \partial_R \theta \mathbf{e}_\theta \otimes \mathbf{E}_R + (r/R) \partial_\Theta \theta \mathbf{e}_\theta \otimes \mathbf{E}_\Theta + [r/(R \sin \Theta)] \partial_\Phi \theta \mathbf{e}_\theta \otimes \mathbf{E}_\Phi \\ &\quad + r \sin \theta \partial_R \phi \mathbf{e}_\phi \otimes \mathbf{E}_R + (r/R) \sin \theta \partial_\Theta \phi \mathbf{e}_\phi \otimes \mathbf{E}_\Theta + [r \sin \theta / (R \sin \Theta)] \partial_\Phi \phi \mathbf{e}_\phi \otimes \mathbf{E}_\Phi. \end{aligned} \quad (\text{B.32})$$

Inverse deformation $\mathbf{X} = \mathbf{X}(\mathbf{x})$ is of the form, in spherical coordinates,

$$R = R(r, \theta, \phi), \quad \Theta = \Theta(r, \theta, \phi), \quad \Phi = \Phi(r, \theta, \phi). \quad (\text{B.33})$$

Referred to natural bases $\{\mathbf{G}_A, \mathbf{g}^a\}$, the inverse deformation gradient is

$$\begin{aligned} \mathbf{F}^{-1} &= \partial_a \mathbf{X} \otimes \mathbf{g}^a = \partial_a X^A \mathbf{G}_A \otimes \mathbf{g}^a = F^{-1A}{}_{.a} \mathbf{G}_A \otimes \mathbf{g}^a \\ &= \partial_r R \mathbf{G}_R \otimes \mathbf{g}^r + \partial_\theta R \mathbf{G}_R \otimes \mathbf{g}^\theta + \partial_\phi R \mathbf{G}_R \otimes \mathbf{g}^\phi \\ &\quad + \partial_r \Theta \mathbf{G}_\Theta \otimes \mathbf{g}^r + \partial_\theta \Theta \mathbf{G}_\Theta \otimes \mathbf{g}^\theta + \partial_\phi \Theta \mathbf{G}_\Theta \otimes \mathbf{g}^\phi \\ &\quad + \partial_r \Phi \mathbf{G}_\Phi \otimes \mathbf{g}^r + \partial_\theta \Phi \mathbf{G}_\Phi \otimes \mathbf{g}^\theta + \partial_\phi \Phi \mathbf{G}_\Phi \otimes \mathbf{g}^\phi. \end{aligned} \quad (\text{B.34})$$

The inverse of the Jacobian determinant $J^{-1} = 1/J$ is

$$J^{-1} = dV/dv = \det[F^{-1A}{}_{.a}] \sqrt{G/g} = \det[\partial_a X^A] [R^2 \sin \Theta / (r^2 \sin \theta)]. \quad (\text{B.35})$$

With respect to orthonormal bases $\{\mathbf{e}_a, \mathbf{E}_A\}$, the inverse deformation gradient is

$$\begin{aligned} \mathbf{F}^{-1} &= F^{-1}{}_{\langle Aa \rangle} \mathbf{E}_A \otimes \mathbf{e}_a \\ &= \partial_r R \mathbf{E}_R \otimes \mathbf{e}_r + (1/r) \partial_\theta R \mathbf{E}_R \otimes \mathbf{e}_\theta + [1/(r \sin \theta)] \partial_\phi R \mathbf{E}_R \otimes \mathbf{e}_\phi \\ &\quad + R \partial_r \Theta \mathbf{E}_\Theta \otimes \mathbf{e}_r + (R/r) \partial_\theta \Theta \mathbf{E}_\Theta \otimes \mathbf{e}_\theta + [R/(r \sin \theta)] \partial_\phi \Theta \mathbf{E}_\Theta \otimes \mathbf{e}_\phi \\ &\quad + R \sin \Theta \partial_r \Phi \mathbf{E}_\Phi \otimes \mathbf{e}_r + (R/r) \sin \Theta \partial_\theta \Phi \mathbf{E}_\Phi \otimes \mathbf{e}_\theta \\ &\quad + [R \sin \Theta / (r \sin \theta)] \partial_\phi \Phi \mathbf{E}_\Phi \otimes \mathbf{e}_\phi. \end{aligned} \quad (\text{B.36})$$

A spatial displacement field in physical spherical coordinates can be constructed using the shifter of (B.17):

$$\begin{aligned} \mathbf{u} &= \mathbf{x} - \mathbf{X} = r \mathbf{g}_r - R \mathbf{G}_R = r \mathbf{g}_r - R g_R^a \mathbf{g}_a \\ &= [r - R g_R^r] \mathbf{e}_r + [-R r g_R^\theta] \mathbf{e}_\theta + [-R r \sin \theta g_R^\phi] \mathbf{e}_\phi = u_r \mathbf{e}_r + u_\theta \mathbf{e}_\theta + u_\phi \mathbf{e}_\phi. \end{aligned} \quad (\text{B.37})$$

The divergence of a second-order tensor field $\mathbf{A}(\mathbf{x}) = A_{\langle ab \rangle} \mathbf{e}_a \otimes \mathbf{e}_b$ in physical spherical coordinates is [65]

$$\begin{aligned} \nabla \cdot \mathbf{A} &= \{(1/r^2) \partial_r (r^2 A_{rr}) + [1/(r \sin \theta)] \partial_\theta (\sin \theta A_{\theta r}) \\ &\quad + [1/(r \sin \theta)] \partial_\phi A_{\phi r} - (1/r) (A_{\theta\theta} + A_{\phi\phi})\} \mathbf{e}_r \\ &\quad + \{(1/r^2) \partial_r (r^2 A_{r\theta}) + [1/(r \sin \theta)] \partial_\theta (\sin \theta A_{\theta\theta}) \\ &\quad + [1/(r \sin \theta)] \partial_\phi A_{\phi\theta} + (1/r) (A_{\theta r} - \cot \theta A_{\phi\phi})\} \mathbf{e}_\theta \\ &\quad + \{(1/r^2) \partial_r (r^2 A_{r\phi}) + (1/r) \partial_\theta (\sin \theta A_{\theta\phi}) \\ &\quad + [1/(r \sin \theta)] \partial_\phi A_{\phi\phi} + (1/r) (A_{\phi r} + A_{\phi\theta})\} \mathbf{e}_\phi. \end{aligned} \quad (\text{B.38})$$

Appendix C: elastic potentials

Let $\mathbf{F} = \nabla_0 \mathbf{x}$ denote the deformation gradient. Eulerian strain \mathbf{D} and Lagrangian Green strain \mathbf{E} , both referred to material coordinates, are defined as [16, 28, 29, 85]

$$\mathbf{D} = \frac{1}{2} (\mathbf{1} - \mathbf{F}^{-1} \mathbf{F}^{-T}), \quad \mathbf{E} = \frac{1}{2} (\mathbf{F}^T \mathbf{F} - \mathbf{1}). \quad (\text{C.1})$$

For a homogeneous material, strain energy per unit reference volume is of the form

$$W = W(\mathbf{F}) = \hat{W}[\mathbf{D}(\mathbf{F})] = \bar{W}[\mathbf{E}(\mathbf{F})]. \quad (\text{C.2})$$

First Piola-Kirchhoff stress and static linear momentum balance in the absence of body force are

$$\mathbf{P} = \partial W / \partial \mathbf{F}, \quad \nabla_0 \cdot \mathbf{P} = \mathbf{0} \quad (\nabla_{0A} P^{aA} = 0). \quad (\text{C.3})$$

Thermodynamic conjugates to strains are symmetric stresses in material coordinates

$$\hat{\mathbf{S}} = \partial \hat{W} / \partial \mathbf{D}, \quad \bar{\mathbf{S}} = \partial \bar{W} / \partial \mathbf{E}. \quad (\text{C.4})$$

From symmetries of tensors in (C.4), the chain rule and $\partial F^{-1A} / \partial F^b_B = -F^{-1A} F^{-1B}{}_{,a}$,

$$\mathbf{P} = \frac{\partial \hat{W}}{\partial \mathbf{D}} : \frac{\partial \mathbf{D}}{\partial \mathbf{F}} = \mathbf{F}^{-T} \hat{\mathbf{S}} \mathbf{F}^{-1} \mathbf{F}^{-T}, \quad \mathbf{P} = \frac{\partial \bar{W}}{\partial \mathbf{E}} : \frac{\partial \mathbf{E}}{\partial \mathbf{F}} = \mathbf{F} \bar{\mathbf{S}}. \quad (\text{C.5})$$

Cauchy stress then follows as [16, 28, 29, 85]

$$\boldsymbol{\sigma} = J^{-1} \mathbf{P} \mathbf{F}^T = J^{-1} \mathbf{F}^{-T} \hat{\mathbf{S}} \mathbf{F}^{-1} = J^{-1} \mathbf{F} \bar{\mathbf{S}} \mathbf{F}^T. \quad (\text{C.6})$$

Using Greek indices to denote Voigt notation in a Cartesian frame (e.g., $\alpha = 1, 2, \dots, 6$), strain energies are written as Taylor polynomials in either strain measure:

$$\hat{W} = \frac{1}{2} \hat{C}_{\alpha\beta} D_\alpha D_\beta + \frac{1}{6} \hat{C}_{\alpha\beta\gamma} D_\alpha D_\beta D_\gamma + \dots, \quad (\text{C.7})$$

$$\bar{W} = \frac{1}{2} \bar{C}_{\alpha\beta} E_\alpha E_\beta + \frac{1}{6} \bar{C}_{\alpha\beta\gamma} E_\alpha E_\beta E_\gamma + \dots. \quad (\text{C.8})$$

Setting moduli $\partial^2 \hat{W} / \partial \mathbf{F} \partial \mathbf{F} = \partial^2 \bar{W} / \partial \mathbf{F} \partial \mathbf{F}$ at the unstrained reference state, second-order elastic constants are equivalent among Eulerian and Lagrangian representations:

$$\hat{C}_{\alpha\beta} = \bar{C}_{\alpha\beta} = C_{\alpha\beta}. \quad (\text{C.9})$$

Setting moduli $\partial^3 \hat{W} / \partial \mathbf{F} \partial \mathbf{F} \partial \mathbf{F} = \partial^3 \bar{W} / \partial \mathbf{F} \partial \mathbf{F} \partial \mathbf{F}$ at the unstrained reference state, third-order elastic constants are related as follows in Cartesian tensor notation [16]:

$$\begin{aligned} \hat{C}_{IJKLMN} = & \bar{C}_{IJKLMN} + \delta_{IK} C_{JLMN} + \delta_{IL} C_{JKMN} + \delta_{IM} C_{KLJN} + \delta_{IN} C_{KLJM} \\ & + \delta_{JK} C_{ILMN} + \delta_{JM} C_{INKL} + \delta_{JL} C_{IKMN} + \delta_{JN} C_{IMKL} \\ & + \delta_{KM} C_{IJLN} + \delta_{KN} C_{IJLM} + \delta_{LM} C_{IJKN} + \delta_{LN} C_{IJKM}. \end{aligned} \quad (\text{C.10})$$

Relations identical to (C.9) and (C.10) can also be derived using the expansion $\mathbf{E} = \mathbf{D} + 2\mathbf{D}^2 + \dots$ and equating like terms in \hat{W} and \bar{W} to third order in strain components [66, 90]. For an isotropic solid [14, 81],

$$C_{IJKL} = \lambda \delta_{IJ} \delta_{KL} + \mu (\delta_{IK} \delta_{JL} + \delta_{IL} \delta_{JK}), \quad (\text{C.11})$$

$$\begin{aligned} \hat{C}_{IJKLMN} = & \hat{\nu}_1 [\delta_{IJ} \delta_{KL} \delta_{MN}] \\ & + \hat{\nu}_2 [\delta_{IJ} (\delta_{KM} \delta_{LN} + \delta_{KN} \delta_{LM}) \\ & + \delta_{KL} (\delta_{IM} \delta_{JN} + \delta_{IN} \delta_{JM}) + \delta_{MN} (\delta_{IK} \delta_{JL} + \delta_{IL} \delta_{JK})] \\ & + \hat{\nu}_3 [\delta_{IK} (\delta_{JM} \delta_{LN} + \delta_{JN} \delta_{LM}) + \delta_{JL} (\delta_{IM} \delta_{KN} + \delta_{IN} \delta_{KM}) \\ & + \delta_{IL} (\delta_{JM} \delta_{KN} + \delta_{JN} \delta_{KM}) + \delta_{JK} (\delta_{IM} \delta_{LN} + \delta_{IN} \delta_{LM})], \end{aligned} \quad (\text{C.12})$$

$$\begin{aligned} \bar{C}_{IJKLMN} = & \bar{\nu}_1 [\delta_{IJ} \delta_{KL} \delta_{MN}] \\ & + \bar{\nu}_2 [\delta_{IJ} (\delta_{KM} \delta_{LN} + \delta_{KN} \delta_{LM}) \\ & + \delta_{KL} (\delta_{IM} \delta_{JN} + \delta_{IN} \delta_{JM}) + \delta_{MN} (\delta_{IK} \delta_{JL} + \delta_{IL} \delta_{JK})] \\ & + \bar{\nu}_3 [\delta_{IK} (\delta_{JM} \delta_{LN} + \delta_{JN} \delta_{LM}) + \delta_{JL} (\delta_{IM} \delta_{KN} + \delta_{IN} \delta_{KM}) \\ & + \delta_{IL} (\delta_{JM} \delta_{KN} + \delta_{JN} \delta_{KM}) + \delta_{JK} (\delta_{IM} \delta_{LN} + \delta_{IN} \delta_{LM})]. \end{aligned} \quad (\text{C.13})$$

These also apply pointwise in a physical components in an orthogonal system, and contravariant components can be recovered for general curvilinear systems by setting $\delta_{IJ} \rightarrow G^{IJ}$. Second-order constants obey the familiar relations

$$C_{11} = \lambda + 2\mu, \quad C_{12} = \lambda, \quad C_{44} = \mu; \quad \nu = \lambda/(2\lambda + 2\mu), \quad K = \lambda + \frac{2}{3}\mu. \quad (\text{C.14})$$

Third-order constants obey the following relations ($\hat{C}_{\alpha\beta\gamma}$ or $\bar{C}_{\alpha\beta\gamma}$):

$$\begin{aligned} C_{111} &= \nu_1 + 6\nu_2 + 8\nu_3, & C_{112} &= \nu_1 + 2\nu_2, & C_{123} &= \nu_1, \\ C_{144} &= \nu_2, & C_{155} &= \nu_2 + 2\nu_3, & C_{456} &= \nu_3. \end{aligned} \quad (\text{C.15})$$

For isotropic materials, (C.10) reduces to

$$\hat{\nu}_1 = \bar{\nu}_1, \quad \hat{\nu}_2 = \bar{\nu}_2 + 2\lambda, \quad \hat{\nu}_3 = \bar{\nu}_3 + 3\mu. \quad (\text{C.16})$$

For hydrostatic loading ($\boldsymbol{\sigma} = -p\mathbf{1}$, $\mathbf{F} = J^{1/3}\mathbf{1}$), pressure derivative of tangent bulk modulus B at the reference state is [16, 42, 63]

$$B'_0 = (dB/dp)|_{p=0} = -\frac{1}{K}(\hat{\nu}_1 + 2\hat{\nu}_2 + \frac{8}{9}\hat{\nu}_3) + 4 = -\frac{1}{K}(\bar{\nu}_1 + 2\bar{\nu}_2 + \frac{8}{9}\bar{\nu}_3). \quad (\text{C.17})$$

Since typical crystalline solids have $2 < B'_0 < 7$ [45], third-order constants $\hat{C}_{\alpha\beta\gamma}$ are generally smaller in magnitude than $\bar{C}_{\alpha\beta\gamma}$, suggesting that series (C.7) converges faster, i.e., requires fewer higher-order terms for a given accuracy, than (C.8). Under hydrostatic loading, stress-strain constitutive relations degenerate to the following pressure-volume equations of state [16, 84]:

$$p = -\partial\bar{W}/\partial J = \frac{3}{2}K(J^{-7/3} - J^{-5/3})[1 + \frac{3}{4}(B'_0 - 4)(J^{-2/3} - 1)], \quad (\text{Eulerian}) \quad (\text{C.18})$$

$$p = -\partial\bar{W}/\partial J = \frac{3}{2}K(J^{-1/3} - J^{1/3})[1 - \frac{3}{4}B'_0(J^{2/3} - 1)]. \quad (\text{Lagrangian}) \quad (\text{C.19})$$

Birch-Murnaghan equation of state (C.18) is often used to accurately fit hydrostatic and shock compression data to high pressures [11, 45], while Lagrangian equation of state (C.19) is usually deemed less accurate [45]. For an isotropic material also obeying Cauchy's symmetry relations [14, 87],

$$\lambda = \mu = \frac{3}{5}K \Leftrightarrow \nu = \frac{1}{4}, \quad (\text{C.20})$$

$$\bar{\nu}_1 = \bar{\nu}_2 = \bar{\nu}_3 = -\frac{9}{35}KB'_0. \quad (\text{C.21})$$

Applying (C.16) with (C.20) and (C.21),

$$\hat{\nu}_1 = -\frac{9K}{35}B'_0, \quad \hat{\nu}_2 = -\frac{K}{5}(\frac{9}{7}B'_0 - 6), \quad \hat{\nu}_3 = -\frac{K}{5}(\frac{9}{7}B'_0 - 9). \quad (\text{C.22})$$

It is instructive to compare Eulerian D -based theory with Murnaghan's theory [61] based on Almansi strain \mathbf{e} :

$$W = \tilde{W}[\mathbf{e}(\mathbf{F})], \quad \mathbf{e} = \frac{1}{2}(\mathbf{1} - \mathbf{F}^{-T}\mathbf{F}^{-1}). \quad (\text{C.23})$$

Because \mathbf{e} is referred to spatial coordinates and is not rotationally invariant, strain energy \tilde{W} is restricted to isotropic materials, in contrast to \bar{W} . Stresses are [61, 84]

$$\boldsymbol{\sigma} = J^{-1}\mathbf{F}^{-T}\mathbf{F}^{-1}\tilde{\mathbf{S}}, \quad \tilde{\mathbf{S}} = \partial\tilde{W}/\partial\mathbf{e}. \quad (\text{C.24})$$

Typically \tilde{W} is expressed as a function of three scalar invariants [38, 52, 61]:

$$\tilde{W}(I_1, I_2, I_3) = (\frac{1}{2}\lambda + \mu)I_1^2 - 2\mu I_2 + \frac{1}{6}(\tilde{\nu}_1 + 6\tilde{\nu}_2 + 8\tilde{\nu}_3)I_1^3 - 2(\tilde{\nu}_2 + 2\tilde{\nu}_3)I_1 I_2 + 4\tilde{\nu}_3 I_3; \quad (\text{C.25})$$

$$I_1 = \text{tr} \mathbf{e}, \quad I_2 = \frac{1}{2}[(\text{tr} \mathbf{e})^2 - \text{tr}(\mathbf{e}^2)], \quad I_3 = \det \mathbf{e}. \quad (\text{C.26})$$

Second-order constants λ and μ are identical to those already introduced. Third-order constants are usually related to Lagrangian constants by writing \bar{W} in terms of invariants of \mathbf{E} , using algebraic relationships between these invariants and those in (C.26) [61], and comparing coefficients of like terms in \tilde{W} and \bar{W} , giving [38]

$$\tilde{\nu}_1 = \frac{1}{3}(\bar{\nu}_1 + 18\bar{\nu}_2 + 44\bar{\nu}_3), \quad \tilde{\nu}_2 = 2(\lambda - \bar{\nu}_2 - 3\bar{\nu}_3), \quad \tilde{\nu}_3 = \bar{\nu}_3 + 3\mu. \quad (\text{C.27})$$

From (C.16) and (C.27), in general $\tilde{\nu}_1 \neq \hat{\nu}_1$ and $\tilde{\nu}_2 \neq \hat{\nu}_2$, but $\tilde{\nu}_3 = \hat{\nu}_3$. These differences arise because of different truncations used to relate Eulerian to Lagrangian strain components or invariants. Note that when \mathbf{F} (and hence \mathbf{F}^{-1}) is symmetric, $\mathbf{D} = \mathbf{e}$ in a common coordinate frame, and \mathbf{D} and \mathbf{e} share the same invariants regardless of rotation. Therefore, for an isotropic solid subjected to a given \mathbf{F} , setting $\tilde{\nu}_1 = \hat{\nu}_1$, $\tilde{\nu}_2 = \hat{\nu}_2$, and $\tilde{\nu}_3 = \hat{\nu}_3$ will produce $\tilde{W} = \hat{W}$ and result in the same Cauchy stress $\boldsymbol{\sigma}$ from (C.24) or the second of (C.6), though generally $\tilde{\mathbf{S}} \neq \hat{\mathbf{S}}$. A Birch-Murnaghan equation of state also follows, i.e., $p = -\partial\tilde{W}/\partial J$ reduces to (C.18). However, because their third-order constants are not required to be equal, in general, energy and stress predicted by Eulerian theory based on \mathbf{D} and that based on \mathbf{e} can differ, even for isotropic materials, and only \mathbf{D} -based theory can be applied to anisotropic materials, of course removing symmetry restrictions in (C.11) and (C.12).

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